```
=> s glorius f?/au
L65         24 GLORIUS F?/AU

=> s L65 and L50
L66          6 L65 AND L50

=> s L65 and L63
L67          4 L65 AND L63

=> s L66 and L67
L68          3 L66 AND L67

=> s L66 or L50
L69         63 L66 OR L50

=> d his

     (FILE 'HOME' ENTERED AT 09:32:44 ON 28 JUN 2006)

     FILE 'REGISTRY' ENTERED AT 09:32:52 ON 28 JUN 2006
L1      1650308 S NCNC2/ESS

     FILE 'REGISTRY' ENTERED AT 09:51:45 ON 28 JUN 2006
L2              STRUCTURE UPLOADED
L3           8980 S L2 FULL
L4              STRUCTURE UPLOADED
L5           3519 S L4 FULL
L6             50 S L4
L7             50 S L2
                SAVE TEMP L5 GLOR800STR2/A

     FILE 'HCAPLUS' ENTERED AT 10:08:22 ON 28 JUN 2006
L8            253 S L5

     FILE 'REGISTRY' ENTERED AT 10:08:52 ON 28 JUN 2006
L9            628 S NC>1 AND L5

     FILE 'STNGUIDE' ENTERED AT 10:12:24 ON 28 JUN 2006

     FILE 'REGISTRY' ENTERED AT 10:14:37 ON 28 JUN 2006
L10             STRUCTURE UPLOADED
L11            50 S L10 SAM SSS  SUB=L5
L12          1426 S L10 FULL SSS  SUB=L5

     FILE 'HCAPLUS' ENTERED AT 10:17:32 ON 28 JUN 2006
L13           108 S L12

     FILE 'REGISTRY' ENTERED AT 10:17:46 ON 28 JUN 2006
L14           237 S L12 AND NRRS>2

     FILE 'HCAPLUS' ENTERED AT 10:27:31 ON 28 JUN 2006
L15            56 S L14

     FILE 'REGISTRY' ENTERED AT 10:27:55 ON 28 JUN 2006
L16          1189 S L12 NOT L14

     FILE 'HCAPLUS' ENTERED AT 10:28:11 ON 28 JUN 2006
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L17          60 S L16
L18           8 S L15 AND L17

     FILE 'REGISTRY' ENTERED AT 10:29:05 ON 28 JUN 2006

     FILE 'STNGUIDE' ENTERED AT 10:29:18 ON 28 JUN 2006

     FILE 'REGISTRY' ENTERED AT 10:45:47 ON 28 JUN 2006
L19             STRUCTURE UPLOADED
L20          32 S L19 SAM SSS  SUB=L12
L21         551 S L19 FULL SSS  SUB=L12

     FILE 'HCAPLUS' ENTERED AT 10:52:12 ON 28 JUN 2006
L22          85 S L21

     FILE 'REGISTRY' ENTERED AT 10:53:23 ON 28 JUN 2006
L23         368 S L21 NOT L14

     FILE 'HCAPLUS' ENTERED AT 10:53:51 ON 28 JUN 2006
L24          45 S L23

     FILE 'REGISTRY' ENTERED AT 10:54:25 ON 28 JUN 2006
L25         875 S L12 NOT L21
L26         821 S L12 NOT (L21 OR L14)
L27        3310 S 180.306.6/RID
L28         809 S L26 AND L27
L29          12 S L26 NOT L28

     FILE 'STNGUIDE' ENTERED AT 11:02:16 ON 28 JUN 2006

     FILE 'REGISTRY' ENTERED AT 11:04:38 ON 28 JUN 2006
L30             STRUCTURE UPLOADED
L31           1 S L30 SAM SSS  SUB=L12
L32          35 S L30 FULL SSS  SUB=L12
L33           0 S L32 AND L24
L34          35 S L32 AND L14

     FILE 'HCAPLUS' ENTERED AT 11:07:03 ON 28 JUN 2006
L35          11 S L34

     FILE 'REGISTRY' ENTERED AT 11:07:31 ON 28 JUN 2006

     FILE 'HCAPLUS' ENTERED AT 11:08:14 ON 28 JUN 2006
L36          54 S L35 OR L24

     FILE 'REGISTRY' ENTERED AT 11:11:52 ON 28 JUN 2006
L37         403 S L23 OR L32

     FILE 'HCAPLUS' ENTERED AT 11:13:36 ON 28 JUN 2006
L38           1 S US2005-520800/APPS
                SEL RN

     FILE 'REGISTRY' ENTERED AT 11:14:26 ON 28 JUN 2006
L39         109 S E1-E109
L40          34 S L39 AND L37
L41          75 S L39 NOT L40
L42           9 S L14 AND L39
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L43          202 S L14 NOT L32

     FILE 'HCAPLUS' ENTERED AT 11:26:41 ON 28 JUN 2006
L44           47 S L43

     FILE 'REGISTRY' ENTERED AT 11:27:00 ON 28 JUN 2006

     FILE 'STNGUIDE' ENTERED AT 11:31:48 ON 28 JUN 2006

     FILE 'REGISTRY' ENTERED AT 11:35:19 ON 28 JUN 2006
L45              STRUCTURE UPLOADED
L46            2 S L45 SAM SSS  SUB=L12
L47           46 S L45 FULL SSS  SUB=L12
L48           46 S L14 AND L47

     FILE 'HCAPLUS' ENTERED AT 11:37:27 ON 28 JUN 2006
L49           12 S L48
L50           63 S L24 OR L35 OR L49

     FILE 'REGISTRY' ENTERED AT 11:38:49 ON 28 JUN 2006
L51          191 S L14 NOT L47
L52          161 S L14 NOT (L47 OR L32)

     FILE 'REGISTRY' ENTERED AT 11:52:20 ON 28 JUN 2006
                SAVE TEMP L23 GLOR800L23/A
                SAVE TEMP L34 GLOR800L34/A
                SAVE TEMP L48 GLOR800L48/A

     FILE 'HCAPLUS' ENTERED AT 11:55:09 ON 28 JUN 2006
                SAVE TEMP L50 GLOR800L50/A

     FILE 'CASREACT' ENTERED AT 12:03:57 ON 28 JUN 2006
L53              STRUCTURE UPLOADED
L54            1 S L53 SAM SSS
L55          113 S L53 FULL SSS
L56           85 S L55/COM
L57              STRUCTURE UPLOADED
L58            1 S L57 SAM SSS
L59            8 S L57 FULL SSS
L60              STRUCTURE UPLOADED
L61            1 S L60
L62           35 S L60 FULL

     FILE 'HCAPLUS' ENTERED AT 12:20:00 ON 28 JUN 2006
L63           35 S L62
L64            3 S L50 AND L63
L65           24 S GLORIUS F?/AU
L66            6 S L65 AND L50
L67            4 S L65 AND L63
L68            3 S L66 AND L67
L69           63 S L66 OR L50

=> file registry
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                               ENTRY    SESSION
FULL ESTIMATED COST                            27.83    1055.64
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FILE COVERS 1907 - 28 Jun 2006 VOL 145 ISS 1
FILE LAST UPDATED: 27 Jun 2006 (20060627/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d ibib abs hitstr L69 1-63

L69 ANSWER 1 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:284758 HCAPLUS
DOCUMENT NUMBER: 145:7488
TITLE: The first palladium-catalyzed Sonogashira coupling of unactivated secondary alkyl bromides
AUTHOR(S): Altenhoff, Gereon; Wuertz, Sebastian; Glorius, Frank
CORPORATE SOURCE: BASF AG, GCB/K-M311, Ludwigshafen, 67056, Germany
SOURCE: Tetrahedron Letters (2006), 47(17), 2925-2928
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

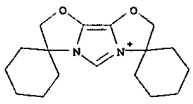
AB A palladium-carbene catalyzed Sonogashira coupling of unactivated alkyl bromides with alkyl substituted alkynes is reported. E.g., [(IBiox7)PdCl2]2 catalyzed the Sonogashira coupling of cycloheptyl bromide with 1-octyne to give 76% 1-octynylcycloheptane. For the first time, unactivated secondary alkyl halides were successfully employed in Sonogashira reactions.

IT 606970-69-8
RL: CAT (Catalyst use); USES (Uses)
(palladium-carbene catalyzed Sonogashira coupling of unactivated alkyl bromides with alkyl substituted alkynes)

RN 606970-69-8 HCAPLUS
CN Dispiro[cyclohexane-1,3'(2'H)-imidazo[5,1-b:4,3-b']bisoxazol[4]ium-7'(8'H),1''-cyclohexane], salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 606970-68-7
CMF C17 H25 N2 O2



CM 2

CRN 37181-39-8
CMF C F3 O3 S

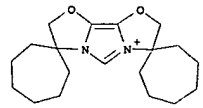
L69 ANSWER 1 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 814254-81-4
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(palladium-carbene catalyzed Sonogashira coupling of unactivated alkyl bromides with alkyl substituted alkynes)

RN 814254-81-4 HCAPLUS
CN Dispiro[cycloheptane-1,3'(2'H)-imidazo[5,1-b:4,3-b']bisoxazol[4]ium-7'(8'H),1''-cycloheptane], salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 814254-80-3
CMF C19 H29 N2 O2



CM 2

CRN 37181-39-8
CMF C F3 O3 S

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:324000 HCAPLUS
DOCUMENT NUMBER: 142:392407
TITLE: Preparation of monocyclic and bicyclic lactams, in particular derivatives of pyrrolidines and pyrroloimidazoles, as Factor Xa inhibitors
INVENTOR(S): Han, Wei; Qiao, Jennifer; Hu, Zilun
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 329 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005032468	A2	20050414	WO 2004-US31857	20040929
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005107361	A1	20050519	US 2004-952397	20040928
EP 1667647	A2	20060614	EP 2004-789189	20040929
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
PRIORITY APPLN. INFO.:			US 2003-507533P	P 20031001
			US 2004-952397	A 20040928
			WO 2004-US31857	W 20040929

OTHER SOURCE(S): MARPAT 142:392407
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. [I and II; V = (CH2)n; n = 1-3; U = (CH2)m; m = 1-2; one of T1 and T2 = CO, CS, SO2, and the other = CO, CS, SO2, CH2, CHOH; one of Z1 and Z2 = N, and the other = C; G = (un)substituted Ph, pyrimidyl, pyrazinyl, pyridazinyl, etc. optionally fused with a 5-6 membered ring containing 0-2 heteroatoms; G1 = SO2NH and derivs., NHCO, NHCSNH and derivs., (un)substituted alkylene, etc.; A = (un)substituted carbocycle, heterocycle; B = alkylene, SO2H and derivs., (un)substituted carbocyle, heterocycle, etc.; R1a at each occurrence = H, (un)substituted alkylene, alkenylene, alkynylene, etc.; or R1aCCR1a = (un)substituted 5-7 membered ring; their stereoisomers or pharmaceutically acceptable salts; with

L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
provisos], were prepd. as inhibitors of trypsin-like serine proteases, specifically Factor Xa. For example, an eleven-step synthesis starting from trans-3-Hydroxy-L-proline is given for lactam III. I displayed Ki ≤ 10 μM for the inhibition of Factor Xa. I were effective thrombin inhibitors; Ki ≤ 10 μM. I are useful antithrombotics.

IT 850001-02-4P, 5-Chlorothiophene-2-carboxylic acid

N-[(7R,7aS)-1-oxo-2-[4-(2-oxo-2H-pyridin-1-yl)phenyl]hexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850001-03-5P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-1-oxo-2-[4-(2-oxopiperidin-1-yl)phenyl]hexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850001-06-8P, 3-Chloro-1H-indole-6-carboxylic acid N-[(7R,7aS)-1-oxo-2-[4-(2-oxo-2H-pyridin-1-yl)phenyl]hexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850001-07-9P, 3-Chloro-1H-indole-6-carboxylic acid N-[(7R,7aS)-1-oxo-2-[4-(3-oxomorpholin-4-yl)phenyl]hexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-06-1P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-1-oxo-2-[4-[1-[2-(pyrrolidin-1-yl)ethyl]cyclobutyl]phenyl]hexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-07-2P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1-(morpholin-4-ylmethyl)cyclobutyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-08-3P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1-[2-(morpholin-4-yl)ethyl]cyclobutyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-09-4P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1-(2-dimethylaminoethyl)cyclopentyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-10-7P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-1-oxo-2-[4-[1-[2-(pyrrolidin-1-yl)ethyl]cyclopropyl]phenyl]hexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-11-8P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1-[2-(morpholin-4-yl)ethyl]cyclopropyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-12-9P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1,1-dimethyl-3-(pyrrolidin-1-yl)propyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-13-0P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1,1-dimethyl-3-(morpholin-4-yl)propyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-14-1P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-(1-methoxymethylcyclopropyl)phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-15-2P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-(1-methoxymethylcyclobutyl)phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-47-0P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-(1-dimethylaminocyclopropyl)phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-48-1P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1-[(dimethylamino)methyl]cyclopropyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-49-2P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1-(2-dimethylaminoethyl)cyclopropyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-50-5P, 5-Chlorothiophene-2-carboxylic acid

N-[(7R,7aS)-2-[4-[1-(carbamoylmethyl)cyclopropyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-51-6P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-(1-dimethylaminocyclobutyl)phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-52-7P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1-[(dimethylamino)methyl]cyclobutyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide 850002-53-8P, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1-(2-

L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

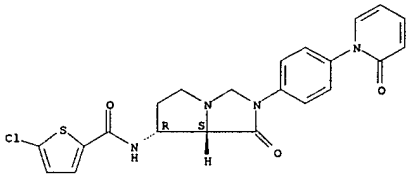
dimethylaminoethyl]cyclobutyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide **850002-54-9P**, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1-(carbamoylmethyl)cyclobutyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide **850002-55-0P**, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-(2-dimethylamino-1,1-dimethylethyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide **850002-56-1P**, 5-Chlorothiophene-2-carboxylic acid

N-[(7R,7aS)-1-oxo-2-[4-[1-(pyrrolidin-1-ylmethyl)cyclopropyl]phenyl]hexahydropyrrolo[1,2-c]imidazol-7-yl]amide **850002-57-2P**, 5-Chlorothiophene-2-carboxylic acid N-[(7R,7aS)-2-[4-[1-(morpholin-4-ylmethyl)cyclopropyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide **850002-58-3P**, 5-Chlorothiophene-2-carboxylic acid

N-[(7R,7aS)-2-[4-[1-[(5-methylthiazol-2-ylamino)methyl]cyclopropyl]phenyl]-1-oxohexahydropyrrolo[1,2-c]imidazol-7-yl]amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; prepn. of monocyclic and bicyclic lactams as Factor Xa inhibitors)

RN 850001-02-4 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-1-oxo-2-[4-(2-oxo-1(2H)-pyridinyl)phenyl]-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

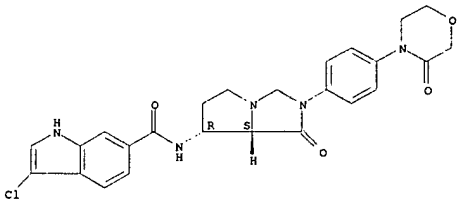
Absolute stereochemistry.



RN 850001-03-5 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-1-oxo-2-[4-(2-oxo-1-piperidinyl)phenyl]-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

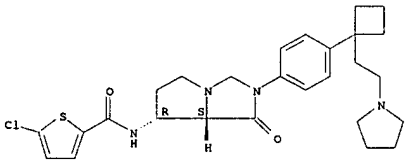
Absolute stereochemistry.

L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



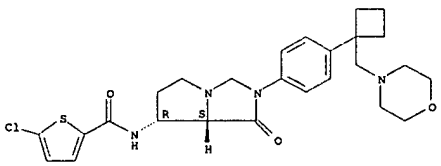
RN 850002-06-1 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-1-oxo-2-[4-[1-[2-(1-pyrrolidinyl)ethyl]cyclobutyl]phenyl]-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

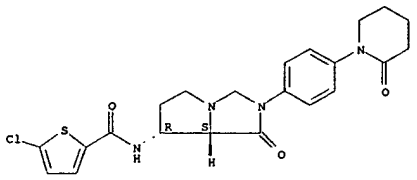


RN 850002-07-2 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-2-[4-[1-(4-morpholinylmethyl)cyclobutyl]phenyl]-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

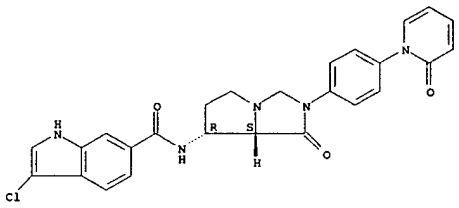


L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 850001-06-8 HCAPLUS
CN 1H-Indole-6-carboxamide, 3-chloro-N-[(7R,7aS)-hexahydro-1-oxo-2-[4-(2-oxo-1(2H)-pyridinyl)phenyl]-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



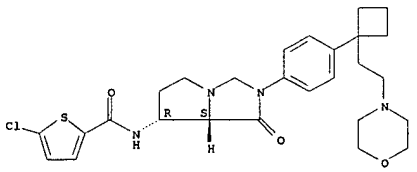
RN 850001-07-9 HCAPLUS
CN 1H-Indole-6-carboxamide, 3-chloro-N-[(7R,7aS)-hexahydro-1-oxo-2-[4-(3-oxo-4-morpholinyl)phenyl]-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

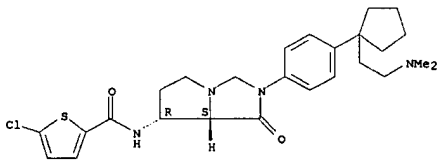
RN 850002-08-3 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-2-[4-[1-[2-(4-morpholinyl)ethyl]cyclobutyl]phenyl]-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 850002-09-4 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-2-[4-[1-[2-(dimethylamino)ethyl]cyclopentyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

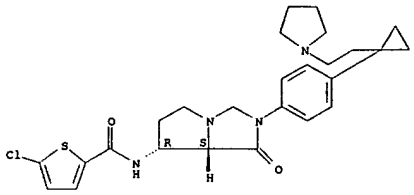
Absolute stereochemistry.



RN 850002-10-7 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-1-oxo-2-[4-[1-[2-(1-pyrrolidinyl)ethyl]cyclopropyl]phenyl]-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

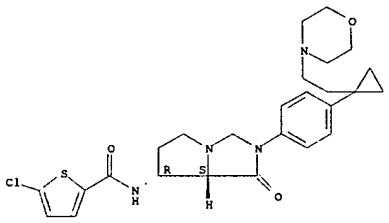
Absolute stereochemistry.

L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 850002-11-8 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-2-[4-[1-[2-(4-morpholinyl)ethyl]cyclopropyl]phenyl]-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

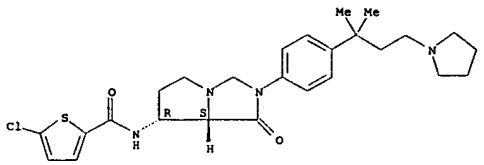
Absolute stereochemistry.



RN 850002-12-9 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-2-[4-[1,1-dimethyl-3-(1-pyrrolidinyl)propyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

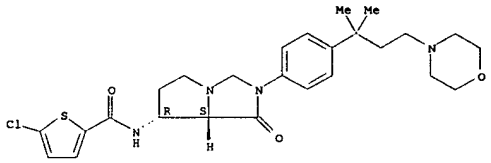
Absolute stereochemistry.

L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



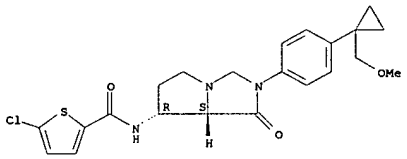
RN 850002-13-0 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-2-[4-[1,1-dimethyl-3-(4-morpholinyl)propyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 850002-14-1 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-2-[4-[1-(methoxymethyl)cyclopropyl]phenyl]-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

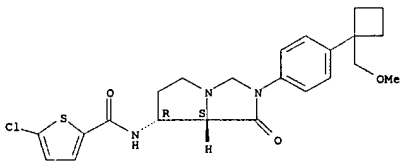
Absolute stereochemistry.



L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

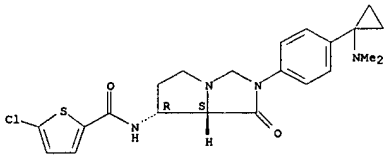
RN 850002-15-2 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-2-[4-[1-(methoxymethyl)cyclobutyl]phenyl]-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



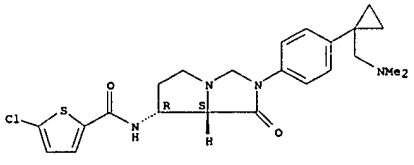
RN 850002-47-0 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-2-[4-[1-(dimethylamino)cyclopropyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 850002-48-1 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-2-[4-[1-[(dimethylamino)methyl]cyclopropyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

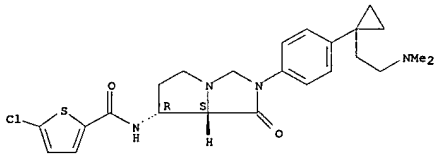
Absolute stereochemistry.



L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

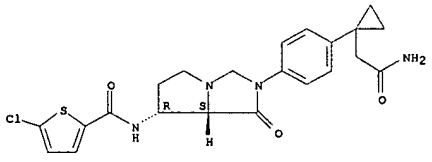
RN 850002-49-2 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-2-[4-[1-[2-(dimethylamino)ethyl]cyclopropyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 850002-50-5 HCAPLUS
CN 2-Thiophenecarboxamide, N-[(7R,7aS)-2-[4-[1-(2-amino-2-oxoethyl)cyclopropyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]-5-chloro- (9CI) (CA INDEX NAME)

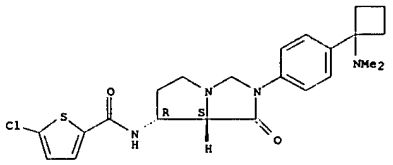
Absolute stereochemistry.



RN 850002-51-6 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-2-[4-[1-(dimethylamino)cyclobutyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

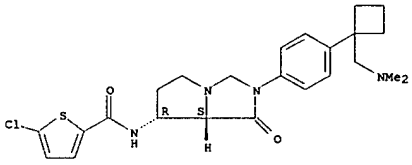
Absolute stereochemistry.

L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



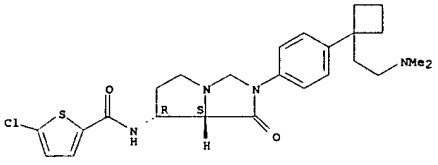
RN 850002-52-7 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-2-[4-[1-[(dimethylamino)methyl]cyclobutyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 850002-53-8 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-2-[4-[1-[2-(dimethylamino)ethyl]cyclobutyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

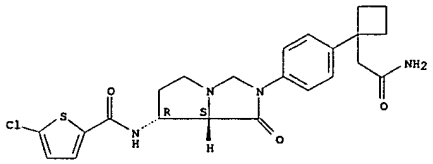
Absolute stereochemistry.



RN 850002-54-9 HCAPLUS

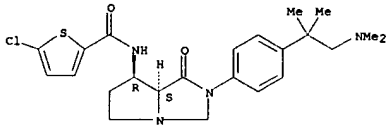
L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 2-Thiophenecarboxamide, N-[(7R,7aS)-2-[4-[1-(2-amino-2-oxoethyl)cyclobutyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]-5-chloro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 850002-55-0 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-2-[4-[2-(dimethylamino)-1,1-dimethylethyl]phenyl]hexahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

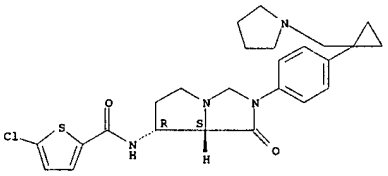
Absolute stereochemistry.



RN 850002-56-1 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-1-oxo-2-[4-[1-(1-pyrrolidinylmethyl)cyclopropyl]phenyl]-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

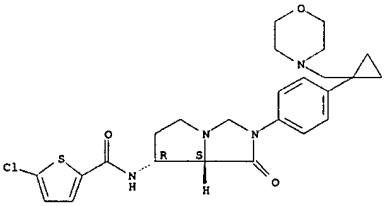
Absolute stereochemistry.

L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 850002-57-2 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-2-[4-[1-(4-morpholinylmethyl)cyclopropyl]phenyl]-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

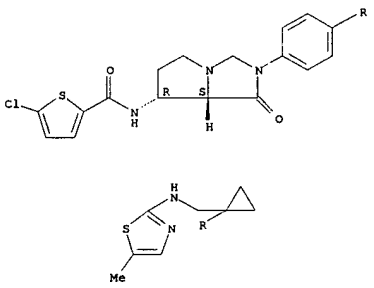
Absolute stereochemistry.



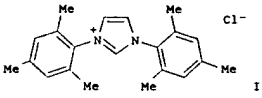
RN 850002-58-3 HCAPLUS
CN 2-Thiophenecarboxamide, 5-chloro-N-[(7R,7aS)-hexahydro-2-[4-[1-[[(5-methyl-2-thiazolyl)amino]methyl]cyclopropyl]phenyl]-1-oxo-1H-pyrrolo[1,2-c]imidazol-7-yl]- (9CI) (CA INDEX NAME)

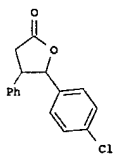
Absolute stereochemistry.

L69 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L69 ANSWER 3 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:1064889 HCAPLUS
DOCUMENT NUMBER: 142:176629
TITLE: Organocatalyzed conjugate umpolung of α,β-unsaturated aldehydes for the synthesis of γ-butyrolactones
AUTHOR(S): Burstein, Christian; Glorius, Frank
CORPORATE SOURCE: Max-Planck-Institut fuer Kohlenforschung, Muelheim an der Ruhr, 45470, Germany
SOURCE: Angewandte Chemie, International Edition (2004), 43(45), 6205-6208
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:176629
GI



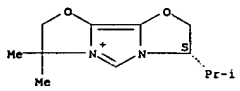


AB N-heterocyclic carbenes can generate homoenolate equivalent under mild conditions by conjugate umpolung of α,β-unsatd. aldehydes. This organocatalytic reaction allows an efficient one-step synthesis of substituted γ-butyrolactones. E.g., the N-heterocyclic carbene generated from imidazolium I was used to catalyze the reaction of (E)-PhCH:CHCHO with 4-ClC6H4CHO to give 53% γ-butyrolactone II (80:20 cis/trans).
IT **832098-68-7**
RL: CAT (Catalyst use); USES (Uses)
(stereoselective preparation of γ-butyrolactones via organocatalyzed conjugate umpolung of α,β-unsatd. aldehydes in reaction with aldehydes or ketones)
RN 832098-68-7 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisoxazol-4-ium, 2,3,7,8-tetrahydro-3,3-dimethyl-7-(1-methylethyl)-, (7S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

L69 ANSWER 3 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CRN 832098-67-6
CMF C12 H19 N2 O2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

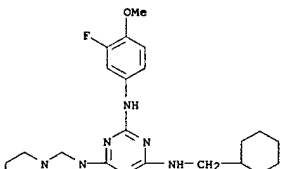
L69 ANSWER 4 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:964820 HCAPLUS
DOCUMENT NUMBER: 141:395584
TITLE: Preparation of novel triazine compounds for inhibiting smooth muscle cell proliferation
INVENTOR(S): Timmer, Richard T.; Alexander, Christopher W.; Pillarisetti, Sivaram; Saxena, Uday; Yeleswarapu, Koteswar Rao; Pal, Manojit; Reddy, Jangalgar Tirupathy; Reddy, Velagala Venkira Rama Murali Krishna; Sridevi, Bhatlapenumarphy Shesha; Kumar, Potlapally Rajender; Reddy, Gaddam Om
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 433 pp., Cont.-in-part of U.S. Ser. No. 390,485.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2004224950	A1	20041111	US 2003-400140		20030326
US 2004077648	A1	20040422	US 2003-390485		20030317
PRIORITY APPLN. INFO.:			US 2001-324147P	P	20010921
			US 2002-253388	B1	20020923
			US 2003-390485	A2	20030317

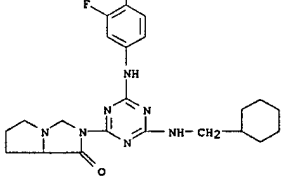
OTHER SOURCE(S): MARPAT 141:395584
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to methods and compns. comprising compds. I or II [R1 = H, alkyl, cycloalkyl, etc.; G = NR1, O; J = CH, N; n = 0-3; X1 = o-R1, m-R1, m-OR1, m-OCF3, etc.; X2 = o-R1, p-R1, p-OR1, p-OCF3, etc.; X3 = o-R1, m-R1, p-R1, o-OR1, p-OR1; or X2 and X3 together is a fused benzene, pyridine, dioxane, tetrahydropyran ring; AY, DY = OR1, F, Cl, Br, I, tetrahydroquinolin-1-yl, etc.; or A, B = O, NR1; and Y = R1, (CHR1)qR1, (CHR1)qCF3, etc.; q = 0-3] that treat pathophysiol. conditions arising from inflammatory responses. Over 100 synthetic examples described synthesis of compds. I and II and their intermediates. E.g., a multi-step synthesis of the triazine III, starting from cyanuric chloride, is given. In particular, the present invention is directed to compds. that inhibit or block glycated protein produced induction of the signaling-associated inflammatory response in endothelial cells. The present invention relates to compds. that inhibit smooth muscle cell (SMC) proliferation. Many of the compds. I and II inhibited SMC proliferation by greater than 70%. Also, the most effective compds. I and II showed an 80% decrease in IL-6 secretion in test for AGE-induced inflammatory response detn. In particular, the present invention is directed to compds. that inhibit smooth muscle cell proliferation by modulating HSPGs such as Perlecan. The present invention further relates to the use of compds. to treat vascular occlusive conditions characterized by smooth muscle proliferation such as restenosis and atherosclerosis.
IT **676358-28-4P 676358-97-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel triazine compds. for inhibiting smooth muscle cell proliferation)
RN 676358-28-4 HCAPLUS
CN 1,3,5-Triazine-2,4-diamine, N-(cyclohexylmethyl)-N'-(3-fluoro-4-methoxyphenyl)-6-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)- (9CI) (CA INDEX NAME)



RN 676358-97-7 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[(cyclohexylmethyl)amino]-6-[(3-fluoro-4-methoxyphenyl)amino]-1,3,5-triazin-2-yl]hexahydro- (9CI) (CA INDEX NAME)



L69 ANSWER 4 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L69 ANSWER 5 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:902612 HCAPLUS
DOCUMENT NUMBER: 142:93738
TITLE: Sterically demanding, bioxazoline-derived N-heterocyclic carbene ligands with restricted flexibility for catalysis
AUTHOR(S): Altenhoff, Gereon; Goddard, Richard; Lehmann, Christian W.; Glorius, Frank
CORPORATE SOURCE: Max-Planck-Institut fuer Kohlenforschung, Muelheim an der Ruhr, 45470, Germany
SOURCE: Journal of the American Chemical Society (2004), 126(46), 15195-15201
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:93738
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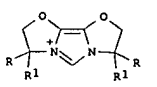

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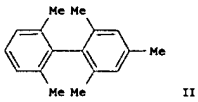


II

AB The triflate salts of imidazobioxazolium ions I [R = R1 = Me; RR1 = (CH2)n; n = 5, 6, 7, 8, 12] are prepared as precursors for sterically demanding and conformationally constrained N-heterocyclic carbene (NHC) ligands; palladium complexes derived from I [RR1 = (CH2)n; n = 7, 12] act as effective catalysts for the Suzuki-Miyaura coupling reactions of ortho-substituted aryl chlorides with ortho-substituted arylboronic acids to provide triortho- and tetraortho-substituted biaryls such as II in 47-96% yields. I•CF3SO3- are prepared in five steps from α,α-disubstituted amino acids and di-Et oxalate; reduction of amino acids to the amino alcs., condensation of the amino alcs. with di-Et oxalate to give the hydroxymethyl-substituted oxamides, chlorination of the primary alc. moieties, cyclization of the oxamide with the chloromethyl groups to give the bioxazolines, and reaction of the bioxazolines with chloromethyl pivalate and silver triflate. I•CF3SO3- are soluble in methylene chloride and THF and are chromatographable. Iridium cyclooctadienyl and iridium dicarbonyl chloride complexes derived from I•CF3SO3- [R = R1 = Me; RR1 = (CH2)n; n = 6, 8 , 12] are prepared; IR frequencies of the carbonyl ligands indicate that carbene ligands derived from I•CF3SO3- are less electron-donating than previous NHC ligands but are comparable to electron-rich phosphines. Selected iridium cyclooctadienyl and iridium dicarbonyl chloride complexes of imidazobioxazolium ligands are characterized by X-ray crystallog. Dimeric palladium chloride complexes derived from I•CF3SO3- [RR1 =

L69 ANSWER 5 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

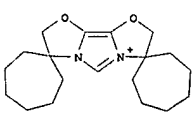
(CH2)n; n = 7 , 12] are prepd. and characterized by X-ray crystallog. Generation of the carbene ligand from I•CF3SO3- [RR1 = (CH2)12] by treatment with potassium hydride and potassium tert-butoxide followed by addn. of palladium acetate yields a palladium catalyst which is effective for the Suzuki-Miyaura coupling of highly hindered aryl chlorides and arylboronic acids. Potassium phosphate is the most effective base and toluene is the most effective solvent for Suzuki-Miyaura coupling of highly hindered aryl chlorides and arylboronic acids using imidazobioxazolium-derived carbene ligands, although cesium carbonate can also be used as the base and 1,4-dioxane as the solvent; the isolated dimeric palladium chloride complexes derived from I•CF3SO3- [RR1 = (CH2)n; n = 7, 12] can also be used as catalysts. Anhyd. conditions are important to minimize hydrodeborylation byproducts of the coupling reaction. E.g., in the presence of the palladium catalyst generated from I•CF3SO3- [RR1 = (CH2)12] and palladium acetate and potassium phosphate, 2-chloro-1,3-dimethylbenzene and 2,4,6-trimethylphenylboronic acid undergo coupling in toluene at 100° for 16 h to provide biphenyl II in 96% yield.

IT **814254-81-4P 814254-83-6P**
RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation and crystal structure of an imidazobioxazolium triflate and its use as a precursor for a sterically hindered and electron-donating N-heterocyclic carbene ligand in Suzuki-Miyaura coupling reactions of hindered aryl chlorides)

RN 814254-81-4 HCAPLUS
CN Dispiro[cycloheptane-1,3'(2'H)-imidazo[5,1-b:4,3-b']bisoxazol[4]ium-7'(8'H),1''-cycloheptane], salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 814254-80-3
CMF C19 H29 N2 O2



CM 2

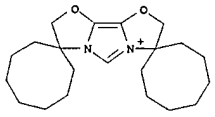
CRN 37181-39-8
CMF C F3 O3 S

L69 ANSWER 5 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 814254-83-6 HCAPLUS
CN Dispiro[cyclooctane-1,3'(2'H)-imidazo[5,1-b:4,3-b']bisoxazol[4]ium-7'(8'H),1''-cyclooctane], salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 814254-82-5
CMF C21 H33 N2 O2



CM 2

CRN 37181-39-8
CMF C F3 O3 S

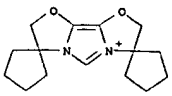
IT **814254-79-0P**
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and crystal structure of an imidazobioxazolium triflate and its use as a precursor for a sterically hindered and electron-donating N-heterocyclic carbene ligand in Suzuki-Miyaura coupling reactions of hindered aryl chlorides)

RN 814254-79-0 HCAPLUS
CN Dispiro[cyclopentane-1,3'(2'H)-imidazo[5,1-b:4,3-b']bisoxazol[4]ium-7'(8'H),1''-cyclopentane], salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 814254-78-9
CMF C15 H21 N2 O2

L69 ANSWER 5 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



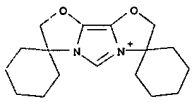
CM 2

CRN 37181-39-8
CMF C F3 O3 S

IT 606970-69-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and crystal structure of an imidazobioxazolium triflate and its
use as a precursor for a sterically hindered and electron-donating N-heterocyclic carbene ligand in Suzuki-Miyaura coupling reactions of hindered aryl chlorides)
RN 606970-69-8 HCAPLUS
CN Dispiro[cyclohexane-1,3'(2'H)-imidazo[5,1-b:4,3-b']bisoxazol[4]ium-7'(8'H),1''-cyclohexane], salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 606970-68-7
CMF C17 H25 N2 O2



CM 2

CRN 37181-39-8

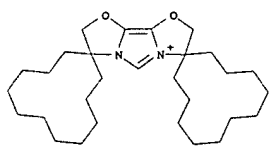
L69 ANSWER 5 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CRN 37181-39-8
CMF C F3 O3 S

IT 814254-85-8P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of an imidazobioxazolium triflate and its use as a precursor
for a sterically hindered and electron-donating N-heterocyclic carbene ligand in Suzuki-Miyaura coupling reactions of hindered aryl chlorides)
RN 814254-85-8 HCAPLUS
CN Dispiro[cyclododecane-1,3'(2'H)-imidazo[5,1-b:4,3-b']bisoxazol[4]ium-7'(8'H),1''-cyclododecane], salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 814254-84-7
CMF C29 H49 N2 O2



CM 2

CRN 37181-39-8
CMF C F3 O3 S

IT 814254-77-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP

L69 ANSWER 5 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CMF C F3 O3 S

IT 814254-86-9
RL: PRP (Properties)
(preparation and crystal structure of an imidazobioxazolium triflate precursor for a sterically hindered and electron-donating N-heterocyclic carbene ligand)
RN 814254-86-9 HCAPLUS
CN Dispiro[cyclododecane-1,3'(2'H)-imidazo[5,1-b:4,3-b']bisoxazol[4]ium-7'(8'H),1''-cyclododecane], salt with trifluoromethanesulfonic acid, compd. with dichloromethane (1:1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 75-09-2
CMF C H2 Cl2

CM 2

CRN 814254-85-8
CMF C29 H49 N2 O2 . C F3 O3 S

CM 3

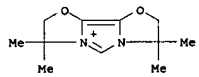
CRN 814254-84-7
CMF C29 H49 N2 O2

CM 4

L69 ANSWER 5 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(Preparation); RACT (Reactant or reagent)
(prepn. of imidazobioxazolium triflates as precursors for sterically hindered and electron-donating N-heterocyclic carbene ligands)
RN 814254-77-8 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisoxazol-4-ium, 2,3,7,8-tetrahydro-3,3,7,7-tetramethyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 814254-76-7
CMF C11 H17 N2 O2



CM 2

CRN 37181-39-8
CMF C F3 O3 S

REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L69 ANSWER 6 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:878154 HCAPLUS
DOCUMENT NUMBER: 141:366254
TITLE: Preparation of novel triazine compounds for inhibiting
smooth muscle cell proliferation
INVENTOR(S): Timmer, Richard T.; Alexander, Christopher W.; Pillarisetti, Sivaram; Saxena, Uday; Yeleswarapu, Koteswar Rao; Pal, Manojit; Reddy, Jangalgar Tirupathy; Krishna, Reddy Velagala Venkata Rama Murali; Sesila, Sridevi Bhatlapenumarthy; Kumar, Potlapally Rajender; Reddy, Gaddam Om
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 422 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2004209882	A1	20041021	US 2003-400169		20030326
US 2005124619	A1	20050609	US 2004-951120		20040927
PRIORITY APPLN. INFO.:			US 2001-324147P	P	20010921
			US 2002-253388	B1	20020923
			US 2003-390485	A2	20030317
			US 2003-400169	A3	20030326

OTHER SOURCE(S): MARPAT 141:366254
GI

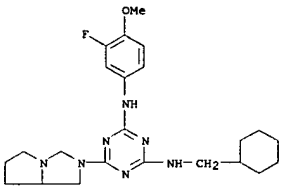
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to methods and compns. comprising compds. I or II [R1 = H, alkyl, cycloalkyl, etc.; G = NR1, O; J = CH, N; n = 0-3; X1 = o-R1, m-R1, m-OR1, m-OCF3, etc.; X2 = o-R1, p-R1, p-OR1, p-OCF3, etc.; X3 = o-R1, m-R1, p-R1, o-OR1, p-OR1; or X2 and X3 together is a fused benzene, pyridine, dioxane, tetrahydropyran ring; AY, DY = OR1, F, Cl, Br, I, tetrahydroquinolin-1-yl, etc.; or A, B = O, NR1; and Y = R1, (CHR1)qR1, (CHR1)qCF3, etc.; q = 0-3] that treat pathophysiol. conditions arising from inflammatory responses. Over 100 synthetic examples described synthesis of compds. I and II and their intermediates. E.g., a multi-step synthesis of the triazine III, starting from cyanuric chloride, is given. In particular, the present invention is directed to compds. that inhibit or block glycated protein produced induction of the signaling-associated

L69 ANSWER 6 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
inflammatory response in endothelial cells. The present invention relates to compds. that inhibit smooth muscle cell (SMC) proliferation. Many of the compds. I and II inhibited SMC proliferation by greater than 70%. Also, the most effective compds. I and II showed an 80% decrease in IL-6 secretion in test for AGE-induced inflammatory response detn. In particular, the present invention is directed to compds. that inhibit smooth muscle cell proliferation by modulating HSPGs such as Perlecan. The present invention further relates to the use of compds. to treat vascular occlusive conditions characterized by smooth muscle proliferation such as restenosis and atherosclerosis.

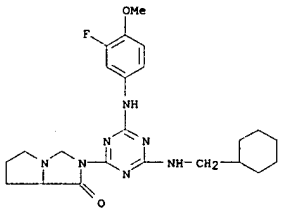
IT **676358-28-4P 676358-97-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel triazine compds. for inhibiting smooth muscle cell proliferation)

RN 676358-28-4 HCAPLUS
CN 1,3,5-Triazine-2,4-diamine, N-(cyclohexylmethyl)-N'-(3-fluoro-4-methoxyphenyl)-6-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)- (9CI) (CA INDEX NAME)



RN 676358-97-7 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[(cyclohexylmethyl)amino]-6-[(3-fluoro-4-methoxyphenyl)amino]-1,3,5-triazin-2-yl]hexahydro- (9CI) (CA INDEX NAME)

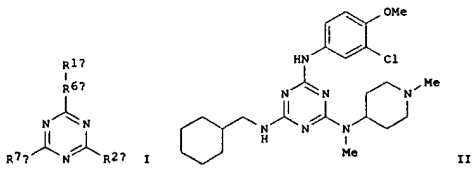
L69 ANSWER 6 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L69 ANSWER 7 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:878153 HCAPLUS
DOCUMENT NUMBER: 141:366253
TITLE: Preparation of novel triazine compounds for inhibiting
smooth muscle cell proliferation
INVENTOR(S): Timmer, Richard T.; Alexander, Christopher W.; Pillarisetti, Sivaram; Saxena, Uday; Yeleswarapu, Koteswar Rao; Pal, Manojit; Reddy, Jangalgar Tirupathy; Krishna, Reddy Velagala Venkata Rama Murali; Sridevi, Bhatlapenumarthy Sesha; Kumar, Potlapally Rajender; Reddy, Gaddam Om
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 254 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

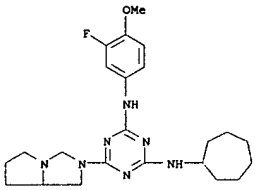
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2004209881	A1	20041021	US 2003-400134		20030326
US 2005113341	A1	20050526	US 2004-951305		20040927
PRIORITY APPLN. INFO.:			US 2001-324147P	P	20010921
			US 2002-253388	B1	20020923
			US 2003-390485	A2	20030317
			US 2003-400134	A3	20030326

OTHER SOURCE(S): MARPAT 141:366253
GI



AB The present invention relates to methods and compns. comprising compds. I [R1b = substituted Ph; R2b = 1-indolyl, substituted NH2, substituted NHMe, substituted OH, etc.; R6b = O, NH, NMe, NEt, N(CN); R7b = cycloheptanyloxy, cyclopropanyloxy, cyclopentanyloxy, cyclohexanyloxy, substituted NH2] that treat pathophysiol. conditions arising from inflammatory responses. Over 100 synthetic examples described synthesis of compds. I and their intermediates. E.g., a multi-step synthesis of the

L69 ANSWER 7 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
triazine II, starting from cyanuric chloride, is given. In particular, the present invention is directed to compds. that inhibit or block glycated protein produced induction of the signaling-assocd. inflammatory response in endothelial cells. The present invention relates to compds. that inhibit smooth muscle cell (SMC) proliferation. Many of the compds. I inhibited SMC proliferation by greater than 70%. In particular, the present invention is directed to compds. that inhibit smooth muscle cell proliferation by modulating HSPGs such as Perlecan. The present invention
further relates to the use of compds. to treat vascular occlusive conditions characterized by smooth muscle proliferation such as restenosis
and atherosclerosis.
IT **676357-62-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel triazine compds. for inhibiting smooth muscle cell
proliferation)
RN 676357-62-3 HCAPLUS
CN 1,3,5-Triazine-2,4-diamine, N-cycloheptyl-N'-(3-fluoro-4-methoxyphenyl)-6-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)- (9CI) (CA INDEX NAME)



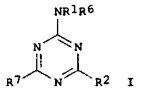
L69 ANSWER 8 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:267312 HCAPLUS
DOCUMENT NUMBER: 140:303704
TITLE: Preparation of aminotriazines for treatment of unwanted cell proliferation, inflammation, hyperproliferation, and as glycosidase modulators.
INVENTOR(S): Timmer, Richard T.; Alexander, Christopher W.; Pillarisetti, Sivaram; Saxena, Uday; Yeleswarapu, Koteswar Rao; Pal, Manojit; Reddy, Jangalgar Tirupathy; Reddy, Velagala Venkata Rama Murali Krishna; Sridevi, Bhatlapenumarthy Sesha; Kumar, Potlapally Rajender; Reddy, Gaddam Om
PATENT ASSIGNEE(S): Reddy US Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 840 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026844	A1	20040401	WO 2003-US9356	20030326
WO 2004026844	C2	20041111		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004077648	A1	20040422	US 2003-390485	20030317
CA 2499964	AA	20040401	CA 2003-2499964	20030326
AU 2003231975	A1	20040408	AU 2003-231975	20030326
BR 2003014670	A	20050809	BR 2003-14670	20030326
EP 1560817	A1	20050810	EP 2003-797788	20030326
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006511476	T2	20060406	JP 2004-538153	20030326

PRIORITY APPLN. INFO.:
US 2002-253388 A 20020923
US 2003-390485 A 20030317
US 2001-324147P P 20010921
WO 2003-US9356 W 20030326

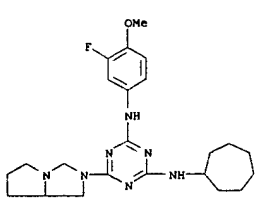
OTHER SOURCE(S): MARPAT 140:303704
GI

L69 ANSWER 8 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



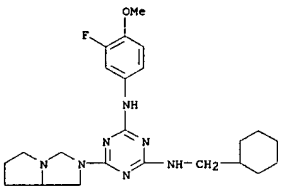
I

AB Title compds. e.g. [I; R1 = substituted Ph, PhCH2, PhCH2CH2, pyridyl; R2 = (substituted) amino, piperazinyl, piperidinyl, thiomorpholinyl, piperidinylamino, hydroxymethylpyrrolidinyl; R6 = H, Me; R7 = hexamethyleneimino, cycloheptylimino, bicyclo[2.2.1]heptyloxy, substituted
amino], were prepared Thus, N2-(3-chloro-4-methoxyphenyl)-N4-cycloheptyl-N6-methyl-N6-piperidin-4-yl-1,3,5-triazine-2,4,6-triamine in an antiproliferation assay (perlican) showed IC50 = 2.2 μM.
IT **676357-62-3P**, N-Cycloheptyl-N'-(3-fluoro-4-methoxyphenyl)-6-(tetrahydropyrrolo[1,2-c]imidazol-2-yl)-[1,3,5]triazine-2,4-diamine **676358-28-4P**, N-Cyclohexylmethyl-N'-(3-fluoro-4-methoxyphenyl)-6-(tetrahydropyrrolo[1,2-c]imidazol-2-yl)-[1,3,5]triazine-2,4-diamine **676358-97-7P**, 2-[4-(Cyclohexylmethylamino)-6-(3-fluoro-4-methoxyphenylamino)-[1,3,5]triazin-2-yl]hexahydropyrrolo[1,2-c]imidazol-1-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminotriazines for treatment of unwanted cell proliferation,
inflammation, hyperproliferation, and as glycosidase modulators)
RN 676357-62-3 HCAPLUS
CN 1,3,5-Triazine-2,4-diamine, N-cycloheptyl-N'-(3-fluoro-4-methoxyphenyl)-6-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)- (9CI) (CA INDEX NAME)

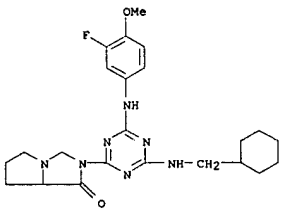


RN 676358-28-4 HCAPLUS
CN 1,3,5-Triazine-2,4-diamine, N-(cyclohexylmethyl)-N'-(3-fluoro-4-methoxyphenyl)-6-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)- (9CI) (CA INDEX NAME)

L69 ANSWER 8 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 676358-97-7 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[(cyclohexylmethyl)amino]-6-((3-fluoro-4-methoxyphenyl)amino]-1,3,5-triazin-2-yl]hexahydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

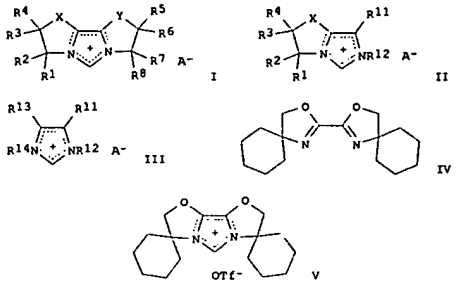
ACCESSION NUMBER: 2004:60481 HCAPLUS
DOCUMENT NUMBER: 140:128420
TITLE: preparation of imidazolium salts from bisimines and alkylating agents in the presence of metal salts as promoters.
INVENTOR(S): Glorius, Frank
PATENT ASSIGNEE(S): Studiengesellschaft Kohle mbH, Germany
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Instant App

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004007465	A1	20040122	WO 2003-DE2285	20030708
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10231368	A1	20040205	DE 2002-10231368	20020711
AU 2003247251	A1	20040202	AU 2003-247251	20030708
EP 1521745	A1	20050413	EP 2003-763695	20030708
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005538071	T2	20051215	JP 2004-520311	20030708
US 2005240025	A1	20051027	US 2005-520800	20050110
PRIORITY APPLN. INFO.:			DE 2002-10231368 A	20020711
			WO 2003-DE2285 W	20030708

OTHER SOURCE(S): MARPAT 140:128420
GI

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB Title compds. [I, II, III; R1-R14 = (unsatd.) (substituted) (cyclic) alkyl, alkenyl, alkynyl, aralkyl, aryl; R1-R8, R11, R13 may addnl. = H; R11, R13 may addnl. = OR16, SR17, NR18R19; R16-R19 = R1; R1, R2, R7, R8, R12, R14, R16-R19 can = linker to another imidazolium residue; X, Y = O, S, (substituted) imino; A = (in)organic (polyvalent) anion] were prepared by reaction of the corresponding bisimines with ZCH2OCO2R15, ZCH2O2CR15, or ZCH2OR15 (Z = leaving group; R15 = R3) in the presence of MA [M = (polyvalent) metal cation, tetraorganoammonium, triorganosilyl; A as above]. Thus, AgOTf and ClCH2O2CCMe3 were stirred 45 min. in CH2Cl2; the resulting solution was added to bisoxazoline (IV) followed by stirring for 20 h at 40° to give 85% title compound (V). V was used as a cocatalyst in Suzuki coupling reactions using sterically hindered aryl chlorides.

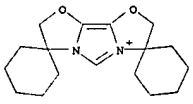
IT **606970-69-8P**
RL: CAT (Catalyst use); IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of imidazolium salts from bisimines and alkylating agents in the presence of metal salts as promoters)

RN 606970-69-8 HCAPLUS
CN Dispiro[cyclohexane-1,3'(2'H)-imidazo[5,1-b:4,3-b']bisoxazol[4]ium-7'(8'H),1''-cyclohexane], salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 606970-68-7
CMF C17 H25 N2 O2

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

CRN 37181-39-8
CMF C F3 O3 S

IT **512193-98-5P 512194-01-3P 512194-04-6P**
648929-49-1P 648929-51-5P 648929-53-7P
648929-57-1P 648929-59-3P 648929-61-7P
648929-63-9P 648929-65-1P 648929-67-3P
648929-69-5P 648929-71-9P 648929-73-1P
648929-75-3P 648929-77-5P 648929-79-7P
648929-81-1P 648929-83-3P 648929-85-5P
648929-87-7P 648929-89-9P 648929-91-3P
648929-93-5P 648929-95-7P 648929-97-9P
648929-99-1P 648930-01-2P 648930-03-4P
648930-05-6P 648930-07-8P 648930-10-3P
648930-12-5P 648930-14-7P 648930-16-9P
648930-18-1P 648930-20-5P 648930-30-7P
648930-34-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of imidazolium salts from bisimines and alkylating agents in the presence of metal salts as promoters)

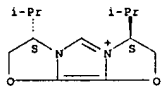
RN 512193-98-5 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisoxazol-4-ium, 2,3,7,8-tetrahydro-3,7-bis(1-methylethyl)-, (3S,7S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 512193-97-4
CMF C13 H21 N2 O2

Absolute stereochemistry. Rotation (+).

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

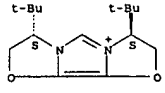
CRN 37181-39-8
CMF C F3 O3 S

RN 512194-01-3 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisoxazol-4-ium, 3,7-bis(1,1-dimethylethyl)-2,3,7,8-tetrahydro-, (3S,7S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 512194-00-2
CMF C15 H25 N2 O2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

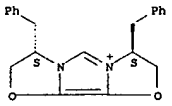
RN 512194-04-6 HCAPLUS

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Imidazo[5,1-b:4,3-b']bisoxazol-4-ium, 2,3,7,8-tetrahydro-3,7-bis(phenylmethyl)-, (3S,7S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 512194-03-5
CMF C21 H21 N2 O2

Absolute stereochemistry.



CM 2

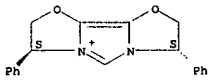
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-49-1 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisoxazol-4-ium, 2,3,7,8-tetrahydro-3,7-diphenyl-, (3S,7S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

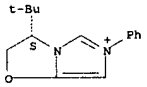
CRN 648929-48-0
CMF C19 H17 N2 O2

Absolute stereochemistry.



CM 2

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.



CM 2

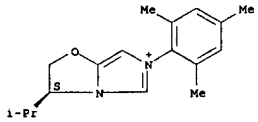
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-57-1 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 2,3-dihydro-3-(1-methylethyl)-6-(2,4,6-trimethylphenyl)-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-56-0
CMF C17 H23 N2 O

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

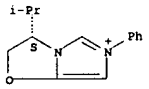
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-51-5 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 2,3-dihydro-3-(1-methylethyl)-6-phenyl-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-50-4
CMF C14 H17 N2 O

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 648929-53-7 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 3-(1,1-dimethylethyl)-2,3-dihydro-6-phenyl-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-52-6
CMF C15 H19 N2 O

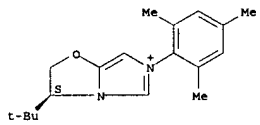
L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 648929-59-3 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 3-(1,1-dimethylethyl)-2,3-dihydro-6-(2,4,6-trimethylphenyl)-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-58-2
CMF C18 H25 N2 O

Absolute stereochemistry.



CM 2

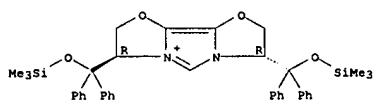
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-61-7 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisoxazol-4-ium, 3,7-bis[diphenyl[(trimethylsilyl)oxy]methyl]-2,3,7,8-tetrahydro-, (3R,7R)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-60-6
CMF C39 H45 N2 O4 Si2

Absolute stereochemistry.



L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

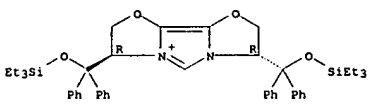
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-63-9 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisoxazol-4-ium, 3,7-bis[diphenyl[(triethylsilyl)oxy]methyl]-2,3,7,8-tetrahydro-, (3R,7R)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-62-8
CMF C45 H57 N2 O4 Si2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 648929-65-1 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6-[2,6-bis(1-methylethyl)phenyl]-2,3-dihydro-3-(1-methylethyl)-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI)

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

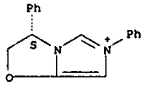
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-69-5 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 2,3-dihydro-3,6-diphenyl-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-68-4
CMF C17 H15 N2 O

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 648929-71-9 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 2,3-dihydro-6-phenyl-3-(phenylmethyl)-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-70-8
CMF C18 H17 N2 O

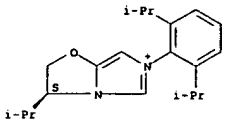
Absolute stereochemistry.

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(CA INDEX NAME)

CM 1

CRN 648929-64-0
CMF C20 H29 N2 O

Absolute stereochemistry.



CM 2

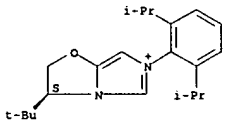
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-67-3 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6-[2,6-bis(1-methylethyl)phenyl]-3-(1,1-dimethylethyl)-2,3-dihydro-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

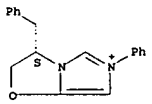
CM 1

CRN 648929-66-2
CMF C21 H31 N2 O

Absolute stereochemistry.



L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

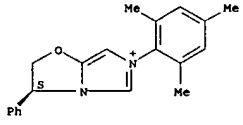
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-73-1 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 2,3-dihydro-3-phenyl-6-(2,4,6-trimethylphenyl)-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-72-0
CMF C20 H21 N2 O

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

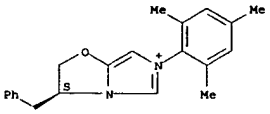
L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 648929-75-3 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 2,3-dihydro-3-(phenylmethyl)-6-(2,4,6-trimethylphenyl)-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-74-2
CMF C21 H23 N2 O

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 648929-77-5 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6-[2,6-bis(1-methylethyl)phenyl]-2,3-dihydro-3-phenyl-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-76-4
CMF C23 H27 N2 O

Absolute stereochemistry.

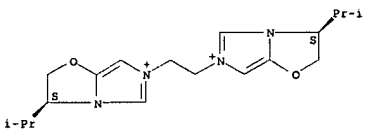
L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 648929-81-1 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,2-ethanediyl)bis[2,3-dihydro-3-(1-methylethyl)-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-80-0
CMF C18 H28 N4 O2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

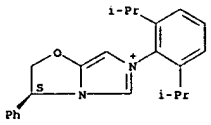
RN 648929-83-3 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,2-ethanediyl)bis[2,3-dihydro-3-(phenylmethyl)-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-82-2
CMF C26 H28 N4 O2

Absolute stereochemistry.

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

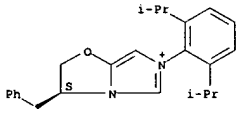
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-79-7 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6-[2,6-bis(1-methylethyl)phenyl]-2,3-dihydro-3-(phenylmethyl)-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-78-6
CMF C24 H29 N2 O

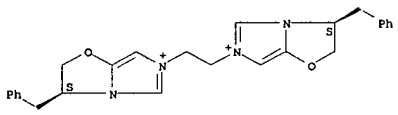
Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

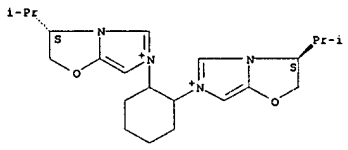
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-85-5 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,2-cyclohexanediyl)bis[2,3-dihydro-3-(1-methylethyl)-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-84-4
CMF C22 H34 N4 O2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

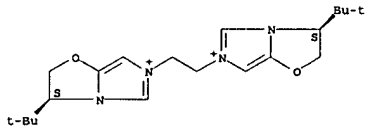
L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 648929-87-7 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,2-ethanediyl)bis[3-(1,1-dimethylethyl)-2,3-dihydro-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-86-6
CMF C20 H32 N4 O2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 648929-89-9 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,2-ethanediyl)bis[2,3-dihydro-3-phenyl-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-88-8
CMF C24 H24 N4 O2

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

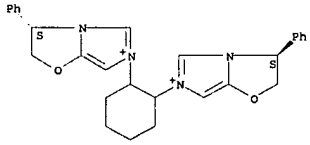
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-93-5 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,2-cyclohexanediyl)bis[2,3-dihydro-3-phenyl-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-92-4
CMF C28 H30 N4 O2

Absolute stereochemistry.



CM 2

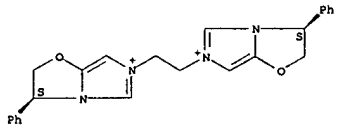
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-95-7 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,3-phenylene)bis[2,3-dihydro-3-(1-methylethyl)-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-94-6
CMF C22 H28 N4 O2

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.



CM 2

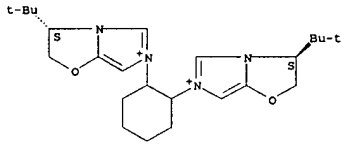
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-91-3 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,2-cyclohexanediyl)bis[3-(1,1-dimethylethyl)-2,3-dihydro-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

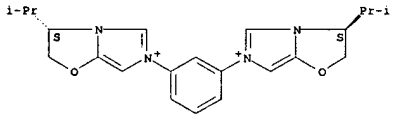
CRN 648929-90-2
CMF C24 H38 N4 O2

Absolute stereochemistry.



CM 2

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.



CM 2

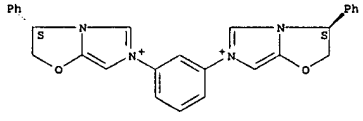
CRN 37181-39-8
CMF C F3 O3 S

RN 648929-97-9 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,3-phenylene)bis[2,3-dihydro-3-phenyl-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-96-8
CMF C28 H24 N4 O2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

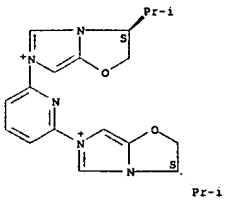
L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 648929-99-1 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(2,6-pyridinediyl)bis[2,3-dihydro-3-(1-methylethyl)-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648929-98-0
CMF C21 H27 N5 O2

Absolute stereochemistry.

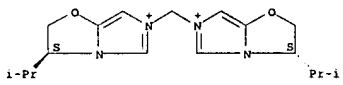


CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 648930-01-2 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(2,6-pyridinediyl)bis[2,3-dihydro-3-phenyl-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

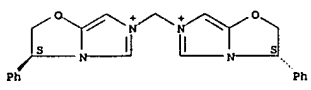
CRN 37181-39-8
CMF C F3 O3 S

RN 648930-05-6 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-methylenebis[2,3-dihydro-3-phenyl-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648930-04-5
CMF C23 H22 N4 O2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

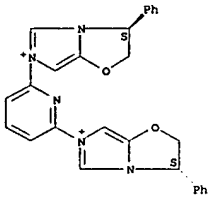
RN 648930-07-8 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,2-cyclohexanediyl)bis[2,3-dihydro-3-(phenylmethyl)-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 1

CRN 648930-00-1
CMF C27 H23 N5 O2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 648930-03-4 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-methylenebis[2,3-dihydro-3-(1-methylethyl)-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648930-02-3
CMF C17 H26 N4 O2

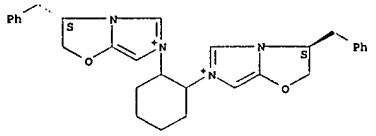
Absolute stereochemistry.

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 1

CRN 648930-06-7
CMF C30 H34 N4 O2

Absolute stereochemistry.



CM 2

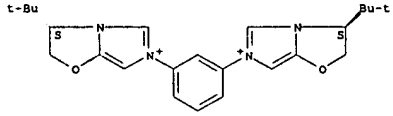
CRN 37181-39-8
CMF C F3 O3 S

RN 648930-10-3 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,3-phenylene)bis[3-(1,1-dimethylethyl)-2,3-dihydro-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648930-09-0
CMF C24 H32 N4 O2

Absolute stereochemistry.



CM 2

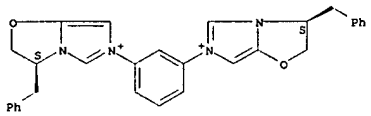
L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CRN 37181-39-8
CMF C F3 O3 S

RN 648930-12-5 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(1,3-phenylene)bis[2,3-dihydro-3-(phenylmethyl)-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648930-11-4
CMF C30 H28 N4 O2

Absolute stereochemistry.



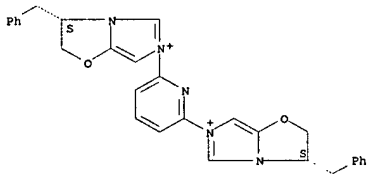
CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 648930-14-7 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(2,6-pyridinediyl)bis[3-(1,1-dimethylethyl)-2,3-dihydro-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

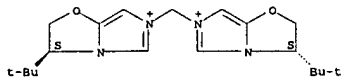
CRN 37181-39-8
CMF C F3 O3 S

RN 648930-18-1 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-methylenebis[3-(1,1-dimethylethyl)-2,3-dihydro-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648930-17-0
CMF C19 H30 N4 O2

Absolute stereochemistry.

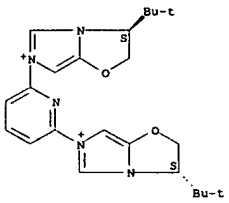


CM 2

CRN 37181-39-8
CMF C F3 O3 S

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CRN 648930-13-6
CMF C23 H31 N5 O2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 648930-16-9 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-(2,6-pyridinediyl)bis[2,3-dihydro-3-(phenylmethyl)-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648930-15-8
CMF C29 H27 N5 O2

Absolute stereochemistry.

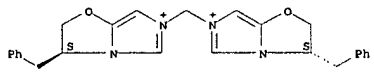
L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 648930-20-5 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6,6'-methylenebis[2,3-dihydro-3-(phenylmethyl)-, (3S,3'S)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 648930-19-2
CMF C25 H26 N4 O2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S

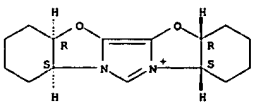
RN 648930-30-7 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisbenzoxazol-11-ium, 1,2,3,4,4a,6a,7,8,9,10,10a,13a-dodecahydro-, (4aR,6aR,10aS,13aS)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648930-29-4
CMF C15 H21 N2 O2

Absolute stereochemistry.

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

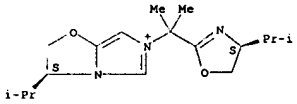
CRN 37181-39-8
CMF C F3 O3 S

RN 648930-34-1 HCAPLUS
CN Imidazo[5,1-b]oxazolium, 6-[1-[(4S)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl]-1-methylethyl]-2,3-dihydro-3-(1-methylethyl)-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 648930-33-0
CMF C17 H28 N3 O2

Absolute stereochemistry.



CM 2

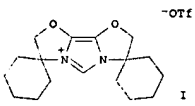
CRN 37181-39-8
CMF C F3 O3 S

L69 ANSWER 9 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L69 ANSWER 10 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:691753 HCAPLUS
DOCUMENT NUMBER: 139:276684
TITLE: An N-heterocyclic carbene ligand with flexible steric bulk allows Suzuki cross-coupling of sterically hindered aryl chlorides at room temperature
AUTHOR(S): Altenhoff, Gereon; Goddard, Richard; Lehmann, Christian W.; **Glorius, Frank**
CORPORATE SOURCE: Max-Planck-Institut fuer Kohlenforschung, Muelheim an der Ruhr, 45470, Germany
SOURCE: Angewandte Chemie, International Edition (2003), 42(31), 3690-3693
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:276684
GI



I

AB A catalyst prepared from Pd(OAc)2 and imidazolium salt I catalyzed the Suzuki cross-coupling of sterically hindered and unhindered, activated and unactivated, aryl chlorides and aryl boronic acids. Obtained were di- and tri-ortho-substituted biphenyl compds.

IT **606970-69-8P**
RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(crystal structure; Suzuki cross-coupling of sterically hindered aryl chlorides and aryl boronic acids catalyzed by catalyst prepared from Pd(OAc)2 and imidazolium salt)

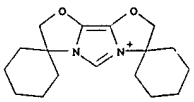
RN 606970-69-8 HCAPLUS
CN Dispiro[cyclohexane-1,3'(2'H)-imidazo[5,1-b:4,3-b']bisoxazol[4]ium-7'(8'H),1''-cyclohexane], salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 606970-68-7
CMF C17 H25 N2 O2

August 11, 2003

L69 ANSWER 10 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

CRN 37181-39-8
CMF C F3 O3 S

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L69 ANSWER 11 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:563667 HCAPLUS
DOCUMENT NUMBER: 140:76926
TITLE: CP0569, A New Broad-Spectrum Injectable Carbapenem. Part 1: Synthesis and Structure-Activity Relationships
AUTHOR(S): Aihara, Kazuhiro; Kano, Yuko; Shiokawa, Sohjiro; Sasaki, Toshiro; Setsu, Fumihito; Sambongi, Yumiko; Ishii, Miyuki; Tohyama, Kazuyo; Ida, Takashi; Tamura, Atsushi; Atsumi, Kunio; Iwamatsu, Katsuyoshi
CORPORATE SOURCE: Pharmaceutical Research Center, Meiji Seika Kaisha, Ltd., Kohoku-ku, Yokohama, 222-8567, Japan
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(16), 3475-3485
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:76926

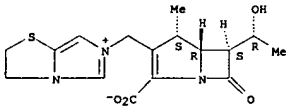
August 5, '03

AB A series of 1β-methylcarbapenems bearing an (imidazo[5,1-b]thiazolium-6-yl)methyl moiety, a 5,5-fused heterobicycle, at the C-2 position was synthesized and evaluated for in vitro antibacterial activities. CP0569 (1r) and its analogs showed potent antibacterial activities against Gram-pos. bacteria, including methicillin-resistant Staphylococcus aureus (MRSA), and Gram-neg. bacteria, including Pseudomonas aeruginosa. Moreover, CP0569 (1r) exhibited stronger antibacterial activity against MRSA and higher resistance to renal dehydropeptidase-1 (DHP-1) than any currently marketed carbapenems, i.e., imipenem (IPM), panipenem (PAPM), and meropenem (MEPM).

IT **640275-17-8P 640275-19-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and structure-activity relationships of carbapenem CP0569)

RN 640275-17-8 HCAPLUS
CN Imidazo[5,1-b]thiazolium, 6-[[(4S,5R,6S)-2-carboxy-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]methyl]-2,3-dihydro-, inner salt (9CI) (CA INDEX NAME)

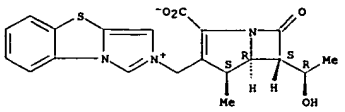
Absolute stereochemistry.



RN 640275-19-0 HCAPLUS
CN Imidazo[5,1-b]benzothiazolium, 2-[[(4S,5R,6S)-2-carboxy-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]methyl]-, inner salt (9CI) (CA INDEX NAME)

L69 ANSWER 11 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L69 ANSWER 12 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:846408 HCAPLUS
DOCUMENT NUMBER: 138:321365
TITLE: Oxazolines as chiral building blocks for imidazolium salts and N-heterocyclic carbene ligands
AUTHOR(S): **Glorius, Frank**; Altenhoff, Gereon; Goddard, Richard; Lehmann, Christian
CORPORATE SOURCE: Max-Planck-Institut fuer Kohlenforschung, Muelheim/Ruhr, 45470, Germany
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (22), 2704-2705
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:321365

after 10/02

AB Enantiomerically pure imidazolium triflates can be readily prepared from bioxazolines and oxazolineimines. Deprotonation of imidazolium triflate gives a chiral N-heterocyclic carbene that can act as a ligand in a catalytically active palladium complex.

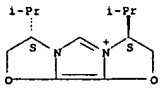
IT **512193-98-5P**
RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation and crystal structure of enantiomerically pure oxazoline-based
imidazolium triflates and their deprotonation to chiral N-heterocyclic carbenes as ligands for palladium-catalyzed arylation reactions)

RN 512193-98-5 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisoxazol-4-ium, 2,3,7,8-tetrahydro-3,7-bis(1-methylethyl)-, (3S,7S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

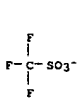
CRN 512193-97-4
CMF C13 H21 N2 O2

Absolute stereochemistry. Rotation (+).



CM 2

CRN 37181-39-8
CMF C F3 O3 S



L69 ANSWER 12 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

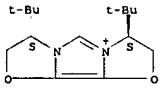
IT **512194-01-3P 512194-04-6P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of enantiomerically pure oxazoline-based imidazolium triflates
and their deprotonation to chiral N-heterocyclic carbenes as ligands for palladium-catalyzed arylation reactions)

RN 512194-01-3 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisoxazol-4-ium, 3,7-bis(1,1-dimethylethyl)-2,3,7,8-tetrahydro-, (3S,7S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

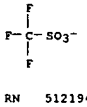
CRN 512194-00-2
CMF C15 H25 N2 O2

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S



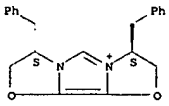
RN 512194-04-6 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisoxazol-4-ium, 2,3,7,8-tetrahydro-3,7-bis(phenylmethyl)-, (3S,7S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 512194-03-5
CMF C21 H21 N2 O2

Absolute stereochemistry.

L69 ANSWER 12 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

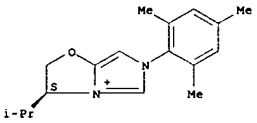
CRN 37181-39-8
CMF C F3 O3 S

IT **512194-12-6P 512194-15-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of enantiomerically pure oxazoline-based imidazolium triflates
and their deprotonation to chiral N-heterocyclic carbenes as ligands for palladium-catalyzed arylation reactions)
RN 512194-12-6 HCAPLUS
CN 2H-Imidazo[5,1-b]oxazol-4-ium, 3,6-dihydro-3-(1-methylethyl)-6-(2,4,6-trimethylphenyl)-, (3S)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 512194-11-5
CMF C17 H23 N2 O

Absolute stereochemistry.



CM 2

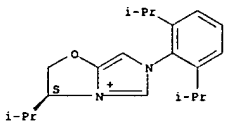
L69 ANSWER 12 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CRN 37181-39-8
CMF C F3 O3 S

RN 512194-15-9 HCAPLUS
CN 2H-Imidazo[5,1-b]oxazol-4-ium, 6-[2,6-bis(1-methylethyl)phenyl]-3,6-dihydro-3-(1-methylethyl)-, (3S)-, salt with trifluoromethanesulfonic acid
(1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 512194-14-8
CMF C20 H29 N2 O

Absolute stereochemistry.



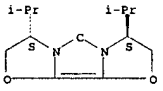
CM 2

CRN 37181-39-8
CMF C F3 O3 S

IT **512194-17-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction with sulfur; preparation of enantiomerically pure oxazoline-based
imidazolium triflates and their deprotonation to chiral N-heterocyclic carbenes as ligands for palladium-catalyzed arylation reactions)

L69 ANSWER 12 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 512194-17-1 HCAPLUS
CN 5H-Imidazo[5,1-b:4,3-b']bisoxazol-5-ylidene, 2,3,7,8-tetrahydro-3,7-bis(1-methylethyl)-, (3S,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



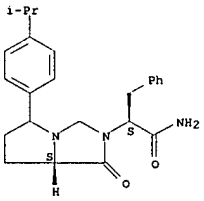
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L69 ANSWER 13 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	2002:379196 HCAPLUS
DOCUMENT NUMBER:	137:201580
TITLE:	An expedient method for the solid-phase synthesis of α-aminoalkyl phosphonopeptides
AUTHOR(S):	Rinnova, Marketa; Nefzi, Adel; Houghten, Richard A.
CORPORATE SOURCE:	Torrey Pines Institute for Molecular Studies, San Diego, CA, 92121, USA
SOURCE:	Tetrahedron Letters (2002), 43(22), 4103-4106 CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER:	Elsevier Science Ltd.
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 137:201580

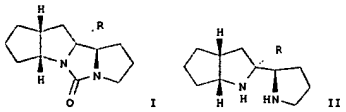
AB The formation of α-amino phosphonate functionalities on the amino terminus of peptides utilizing solid-phase methodol. is presented. The described method enables incorporation of diverse N-phosphonoalkyl and aryl moieties.
IT **453540-91-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of aminoalkyl phosphonopeptides)
RN 453540-91-5 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetamide, tetrahydro-5-[4-(1-methylethyl)phenyl]-1-oxo-α-(phenylmethyl)-, (αS,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



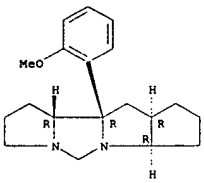
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L69 ANSWER 14 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:87891 HCAPLUS
DOCUMENT NUMBER: 137:6120
TITLE: Highly diastereoselective addition of N-Boc-pyrrolidin-2-yllithium to optically active ketimines - synthesis of enantiomerically pure 1,3-imidazolidin-2-ones and diamines
AUTHOR(S): von Keyserlingk, Nikolai Graf; Martens, Jurgen
CORPORATE SOURCE: Universitat Oldenburg, Fachbereich Chemie, Oldenburg, 26129, Germany
SOURCE: European Journal of Organic Chemistry (2002), (2), 301-308
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:6120
GI



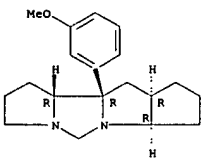
AB A highly diastereoselective addition of chiral N-Boc-pyrrolidin-2-yllithium to optically active bicyclic ketimines has been developed. For this purpose alkyl- and aryl-substituted chiral N-Boc-amino ketones have been synthesized by addition of various Grignard reagents to an N-Boc-protected lactam. The resulting N-Boc-amino ketones have been converted into bicyclic ketimines after deprotection and intramol. cyclization. A kinetic resolution of the racemic organolithium compound by the chiral substrate is discussed based on x-ray crystal structure anal. and exptl. results. The influence of the substituent of the ketimine has been studied. Some of the obtained tetracyclic 1,3-imidazolidin-2-ones I (R = Ph, 4-MeC6H4, 3-MeOC6H4, 2-MeOC6H4) have been converted into tetracyclic aminals and these compds. have been hydrolyzed to the desired diamines II (R = Ph, 4-MeC6H4, 3-MeOC6H4, 2-MeOC6H4).
IT **431887-13-7P 431887-41-1P 431887-43-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(diastereoselective addition of N-Boc-pyrrolidin-2-yllithium to optically active ketimines for synthesis of enantiomerically pure 1,3-imidazolidin-2-ones and diamines and kinetic resolution of the racemic organolithium compound)
RN 431887-13-7 HCAPLUS

L69 ANSWER 14 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT **431887-42-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(diastereoselective addition of N-Boc-pyrrolidin-2-yllithium to optically active ketimines for synthesis of enantiomerically pure 1,3-imidazolidin-2-ones and diamines and kinetic resolution of the racemic organolithium compound)
RN 431887-42-2 HCAPLUS
CN 1H,5H-Cyclopenta[4,5]pyrrolo[1,2-c]pyrrolo[2,1-e]imidazole, decahydro-9b-(3-methoxyphenyl)-, (3aR,9aR,9bR,10aR)- (9CI) (CA INDEX NAME)

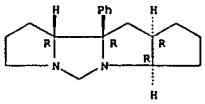
Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

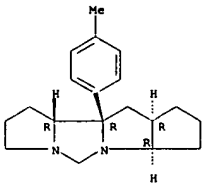
L69 ANSWER 14 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1H,5H-Cyclopenta[4,5]pyrrolo[1,2-c]pyrrolo[2,1-e]imidazole, decahydro-9b-phenyl-, (3aR,9aR,9bR,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 431887-41-1 HCAPLUS
CN 1H,5H-Cyclopenta[4,5]pyrrolo[1,2-c]pyrrolo[2,1-e]imidazole, decahydro-9b-(4-methylphenyl)-, (3aR,9aR,9bR,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



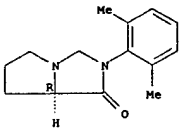
RN 431887-43-3 HCAPLUS
CN 1H,5H-Cyclopenta[4,5]pyrrolo[1,2-c]pyrrolo[2,1-e]imidazole, decahydro-9b-(2-methoxyphenyl)-, (3aR,9aR,9bR,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L69 ANSWER 15 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:905331 HCAPLUS
DOCUMENT NUMBER: 136:241071
TITLE: Increased rigidity of the chiral centre of tocainide favours stereoselectivity and use-dependent block of skeletal muscle Na+ channels enhancing the antimyotonic activity in vivo
AUTHOR(S): Talon, Sophie; De Luca, Annamaria; De Bellis, Michela; Desaphy, Jean-Francois; Lentini, Giovanni; Scilimati, Antonio; Corbo, Filomena; Franchini, Carlo; Tortorella, Paolo; Jockusch, Harald; Camerino, Diana Conte
CORPORATE SOURCE: Department of Pharmacobiology, Unit of Pharmacology, Faculty of Pharmacy, University of Bari, Bari, I-70125, Italy
SOURCE: British Journal of Pharmacology (2001), 134(7), 1523-1531
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 1 Searching for the structural requirements improving the potency and the stereoselectivity of Na+ channel blockers as antimyotonic agents, new derivs. of tocainide, in which the chiral carbon atom is constrained in a rigid α-proline or pyrrolo-imidazolic cycle, were tested as pure enantiomers. 2 Their ability to block Na+ currents, elicited from -100 to -20 mV at 0.3 Hz (tonic block) and 2-10 Hz (use-dependent block) frequencies, was investigated in vitro on single fibers of frog semitendinosus muscle using the vaseline-gap voltage-clamp method. 3 The α-proline derivative, To5, was 5 and 21 fold more potent than tocainide in producing tonic and 10 Hz-use-dependent block, resp. Compared to To5, the presence of one Me group on the aminic (To6) or amidic (To7) nitrogen atom decreased use-dependence by 2- and 6-times, resp. When methylene moieties were present on both nitrogen atoms (To8), both tonic and use-dependent block were reduced. 4 Contrarily to tocainide, all proline derivs. were stereoselective in relation to an increased rigidity. A further increase in the mol. rigidity as in pyrrolo-imidazolic deriv. markedly decreased the drug potency with respect to tocainide. 5 Antimyotonic activity, evaluated as the shortening of the time of righting reflexes of myotonic adr/adr mice upon acute drug in vivo administration was 3 fold more effective for R-To5 than for R-Tocainide. 6 Thus, constraining the chiral center of tocainide in α-proline cycle leads to more potent and stereoselective use-dependent Na+ channel blockers with improved therapeutic potential.
IT **403995-20-0 403995-21-1**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(increased rigidity of the chiral center of tocainide favors stereoselectivity and use-dependent block of skeletal muscle Na+ channels enhancing the antimyotonic activity in vivo)
RN 403995-20-0 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(2,6-dimethylphenyl)hexahydro-, (7aR)- (9CI) (CA INDEX NAME)

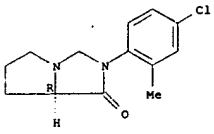
Absolute stereochemistry.

L69 ANSWER 15 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 403995-21-1 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-chloro-2-methylphenyl)hexahydro-, (7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

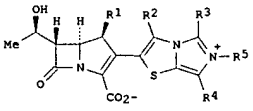


REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L69 ANSWER 16 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:565047 HCAPLUS
DOCUMENT NUMBER: 135:152661
TITLE: Preparation of novel carbapenem derivatives of quaternary salt type as antimicrobial agents
INVENTOR(S): Kano, Yuko; Maruyama, Takahisa; Yamamoto, Yasuo; Shitara, Eiji; Sasaki, Toshiro; Aihara, Kazuhiro; Atsumi, Kunio; Iwamatsu, Katsuyoshi; Ida, Takashi
PATENT ASSIGNEE(S): Meiji Seika Kaisha, Ltd., Japan
SOURCE: PCT Int. Appl., 329 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001055155	A1	20010802	WO 2001-JP529	20010126
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2398478	AA	20010802	CA 2001-2398478	20010126
AU 2001028833	A5	20010807	AU 2001-28833	20010126
EP 1251134	A1	20021023	EP 2001-946865	20010126
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003022881	A1	20030130	US 2002-182180	20020725
US 6825187	B2	20041130		
PRIORITY APPLN. INFO.:			JP 2000-17418 A	20000126
			WO 2001-JP529 W	20010126

OTHER SOURCE(S): MARPAT 135:152661
GI

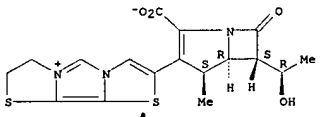


I

L69 ANSWER 16 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
AB Carbapenem derivs. represented by the general formula [I; R1 = H, Me; R2, R3 = H, halo, lower alkyl optionally substituted by HO or NH2, lower alkylcarbonyl, CONH2, aryl, lower alkylthio; R4 = (un)substituted lower alkylthio, lower cycloalkylthio, C2-4 alkenylthio, C2-4 alkynylthio, mono- or bicyclic heterocyclylthio containing ≥1 of same or different heteroatoms, lower alkylsulfinyl, (un)substituted lower alkylsulfonyl, lower alkylcarbonyl, arylcarbonyl; or R4 and R5 are linked to each other to represent S(CH2)n (n = 2-4); R5 = (un)substituted lower alkyl, lower cycloalkyl, C2-4 alkenyl, C2-4 alkynyl, (un)substituted 4- to 7-membered aliphatic heterocyclyl optionally containing ≥1 of O or S atoms] are prepared These compds. have potent antibacterial activities on methicillin-resistant Staphylococcus aureus (MRSA), penicillin-resistant Streptococcus pneumoniae (PRSP), Haemophilus influenzae, and β-lactamase-producing bacteria and a high stability to renal dehydropeptidase enzyme (DHP-1). Thus, (1S,5R,6S)-6-[(1R)-1-hydroxyethyl]-1-methyl-2-(7-methylthioimidazo[5,1-b]thiazol-2-yl)-1-carbapen-2-em-3-carboxylic acid p-nitrobenzyl ester (preparation given) was dissolved in CH2Cl2, cooled in an ice bath, treated with 0.022 mL Me trifluoromethanesulfonate, and stirred at the same temperature for 30 min to give (1S,5R,6S)-6-[(1R)-1-hydroxyethyl]-1-methyl-2-(6-methyl-7-methylthioimidazo[5,1-b]thiazolium-2-yl)-1-carbapen-2-em-3-carboxylic acid p-nitrobenzyl ester trifluoromethanesulfonate which was hydrogenolyzed over 10% Pd-C in a mixture of 1 N phosphate buffer (pH 6.8) and THF under hydrogen atmospheric for 1.5 h to give (1S,5R,6S)-6-[(1R)-1-hydroxyethyl]-1-methyl-2-(6-methyl-7-methylthioimidazo[5,1-b]thiazolium-2-yl)-1-carbapen-2-em-3-carboxylate (inner salt) (II). II in vitro showed min. inhibitory concentration of 1.56 and 0.025 μg/mL against highly methicillin-resistant Staphylococcus aureus M126 and highly penicillin-resistant Streptococcus pneumoniae, resp.
IT **352306-76-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel carbapenem derivs. quaternary salts as antimicrobial agents)
RN 352306-76-4 HCAPLUS
CN Imidazo[5,1-b:4,3-b']bisthiazol-4-ium, 8-[(4S,5R,6S)-2-carboxy-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]-2,3-dihydro-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L69 ANSWER 16 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

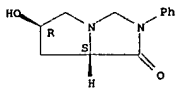


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

double bond

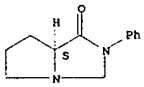
L69 ANSWER 17 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:47298 HCAPLUS
DOCUMENT NUMBER: 134:280528
TITLE: Enantioselective desymmetrization of meso-cyclic anhydrides catalyzed by hexahydro-1H-pyrrolo[1,2-c]imidazolones
AUTHOR(S): Uozumi, Y.; Yasoshima, K.; Miyachi, T.; Nagai, S.-i.
CORPORATE SOURCE: Institute for Molecular Science, Myodaiji, Okazaki, 444-8585, Japan
SOURCE: Tetrahedron Letters (2001), 42(3), 411-414
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:280528
AB Asym. methanolysis of meso cyclic carboxylic anhydrides including hexahydrophthalic anhydride proceeded in toluene in the presence of (6R,7aS)-2-aryl-6-hydroxyhexahydro-1H-pyrrolo[1,2-c]imidazol-1-one to give the corresponding desymmetrized monoester acids, e.g. (1S,2R)-2-(methoxycarbonyl)cyclohexane-1-carboxylic acid, with ≤89% ee.
IT **173549-74-1P 332123-98-5P 332123-99-6P 332943-88-1P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(asym. methanolysis of meso-cyclic anhydrides catalyzed by hexahydropyrrolo[1,2-c]imidazolones)
RN 173549-74-1 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-6-hydroxy-2-phenyl-, (6R,7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 332123-98-5 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-, (7aS)- (9CI) (CA INDEX NAME)

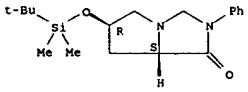
Absolute stereochemistry.



RN 332123-99-6 HCAPLUS

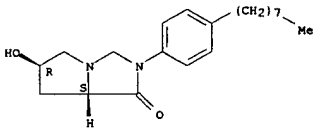
L69 ANSWER 17 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-2-phenyl-, (6R,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 332943-88-1 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-6-hydroxy-2-(4-octylphenyl)-, (6R,7aS)- (9CI) (CA INDEX NAME)

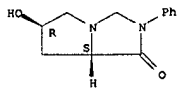
Absolute stereochemistry.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

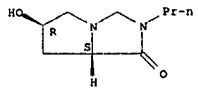
L69 ANSWER 18 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:47297 HCAPLUS
DOCUMENT NUMBER: 134:266218
TITLE: A parallel preparation of a bicyclic N-chiral amine library and its use for chiral catalyst screening
AUTHOR(S): Uozumi, Y.; Mizutani, K.; Nagai, S.-i.
CORPORATE SOURCE: Institute for Molecular Science, Myodaiji, Okazaki, 444-8585, Japan
SOURCE: Tetrahedron Letters (2001), 42(3), 407-410
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:266218
AB A parallel library of optically active bicyclic tertiary amines bearing N-chiral bridgehead nitrogen atoms was readily prepared by condensation of primary amines, cyclic amino acids, and aldehydes. The enantiocontrolling ability of each of the library members was examined for the asym. alkylation of benzaldehyde with diethylzinc, and (3R,6R,7aS)-(2,3-diphenyl-6-hydroxy)hexahydro-1H-pyrrolo[1,2-c]imidazol-1-one, which contains a β-amino alc. unit, showed high enantioselectivity.
IT **173549-74-1P 332123-92-9P 332123-95-2P 332123-96-3P 332123-97-4P 332123-98-5P 332123-99-6P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(parallel preparation of bicyclic N-chiral amine library)
RN 173549-74-1 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-6-hydroxy-2-phenyl-, (6R,7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 332123-92-9 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-6-hydroxy-2-propyl-, (6R,7aS)-(9CI) (CA INDEX NAME)

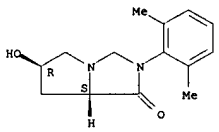
Absolute stereochemistry.



RN 332123-95-2 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(2,6-dimethylphenyl)hexahydro-6-hydroxy-

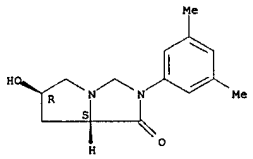
L69 ANSWER 18 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
, (6R,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



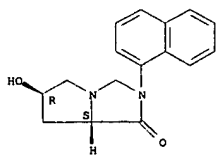
RN 332123-96-3 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(3,5-dimethylphenyl)hexahydro-6-hydroxy-, (6R,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 332123-97-4 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-6-hydroxy-2-(1-naphthalenyl)-, (6R,7aS)- (9CI) (CA INDEX NAME)

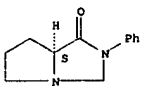
Absolute stereochemistry.



RN 332123-98-5 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-, (7aS)- (9CI) (CA INDEX NAME)

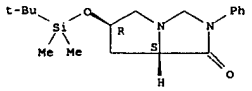
Absolute stereochemistry.

L69 ANSWER 18 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 332123-99-6 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one,
6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]
hexahydro-2-phenyl-, (6R,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

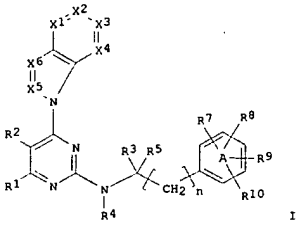
L69 ANSWER 19 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:12273 HCAPLUS
DOCUMENT NUMBER: 134:86271
TITLE: Preparation of pyrimidine derivatives as Src-family protein tyrosine kinase inhibitor compounds
INVENTOR(S): Armstrong, Helen M.; Beresis, Richard; Goulet, Joung L.; Holmes, Mark A.; Hong, Xingfang; Mills, Sander G.; Parsons, William H.; Sinclair, Peter J.; Steiner, Mark G.; Wong, Frederick; Zaller, Dennis M.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 470 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000213	A1	20010104	WO 2000-US17443	20000626
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2383546	AA	20010104	CA 2000-2383546	20000626
EP 1206265	A1	20020522	EP 2000-941701	20000626
EP 1206265	B1	20031112		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
US 6498165	B1	20021224	US 2000-604305	20000626
JP 2003523942	T2	20030812	JP 2001-505922	20000626
AT 253915	E	20031115	AT 2000-941701	20000626
PRIORITY APPLN. INFO.:			US 1999-141639P P	19990630
			WO 2000-US17443 W	20000626

OTHER SOURCE(S): MARPAT 134:86271
GI

L69 ANSWER 19 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



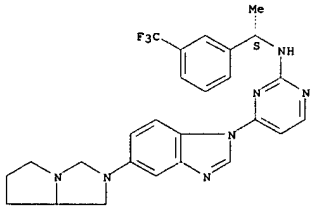
I

AB What are claimed are pyrimidine compds. (shown as I), or their pharmaceutically acceptable salts, hydrates, solvates, crystal forms and individual diastereomers, and pharmaceutical compns. including the same and their use as inhibitors of tyrosine kinase enzymes and consequently their use in the prophylaxis and treatment of protein tyrosine kinase-associated disorders, such as immune diseases, hyperproliferative disorders and other diseases in which inappropriate protein kinase action is believed to play a role, such as cancer, angiogenesis, atherosclerosis, graft rejection, rheumatoid arthritis and psoriasis. In I, R1, R2 = independently H, halo, OH, SH, CN, NO2, alkyl, alkoxy, acyloxy, alkoxycarbonyloxy, carbamoyloxy, alkylthio, sulfinyl, sulfonyl, acyl, alkoxycarbonyl, carbamoyl, amino, acylamino, ureido, sulfamoyl, sulfonylamino, or R1 and R2 can join together to form a fused methylenedioxy ring or a fused 6-membered aromatic ring; terms such as 'alkyl' here and below are further defined in the claims. R3, R5 = independently H, C1-C6-alkyl unsubstituted or substituted with 1-3 substituents, aryl, or R3 and R5 taken together can represent :O; R3 or R5 can represent a 2 or 3 C methylene bridge forming a ring of 5-8 atoms fused to the A ring. R4 = H, C1-C6-alkyl, C1-C6-alkoxyl. X1, X2, X3, X4 in -X1:X2-X3:X4- are substituted or unsubstituted CH or N where 0-2 of X1, X2, X3, X4 are N. X5, X6 = independently N, C, optionally substituted CH. A ring = Ph, naphthyl, pyridyl, pyrazinyl, pyrimidinyl, pyrrolyl, thienyl, oxazolyl, isoxazolyl, thiazolyl, pyrazolyl, triazolyl, tetrazolyl, furanyl, benzothienyl, benzofuranyl, indolyl, imidazolyl, benzimidazolyl, thiadiazolyl. R7, R8, R9, R10 = independently H, halo, OH, SH, CN, NO2, N3, N2+BF4-, alkyl, alkoxy, alkylthio, sulfinyl, sulfonyl, C1-C6-alkyl, C1-C6-perfluoroalkyl, acyl, alkoxycarbonyl, carbamoyl, acyloxy, alkoxycarbonyloxy, carbamoyloxy, amino, acylamino, ureido, sulfamoyl, sulfonylamino, two of R7, R8, R9, and R10 when on adjacent carbons join together to form a methylenedioxy bridge. N = 0-2. More than 500 example preps. are given, but no preparative method is claimed and no data relating to the usefulness of the compds. are given.

IT **317826-43-0P**, 2-[(S)-(3-Trifluoromethylphenyl)ethylamino]-4-[5-(3-diazabicyclo[3.3.0]oct-3-yl)benzimidazol-1-yl]pyrimidine
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of pyrimidine derivs. as Src-family protein tyrosine kinase inhibitor compds.)

RN 317826-43-0 HCAPLUS
CN 2-Pyrimidinamine, 4-[5-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1H-benzimidazol-1-yl]-N-[(1S)-1-[3-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

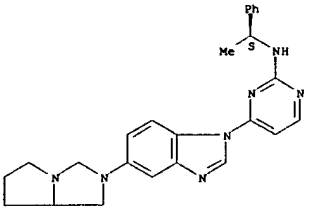


IT **317826-08-7P**, 2-[(S)-1-Phenylethylamino]-4-[5-(1,3-diazabicyclo[3.3.0]oct-3-yl)benzimidazol-1-yl]pyrimidine **317826-09-8P**, 2-[(S)-1-Phenylethylamino]-4-[6-(1,3-diazabicyclo[3.3.0]oct-3-yl)benzimidazol-1-yl]pyrimidine **317826-42-9P**, 2-[(S)-1-(3-Nitrophenyl)ethylamino]-4-[5-(1,3-diazabicyclo[3.3.0]oct-3-yl)benzimidazol-1-yl]pyrimidine
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as Src-family protein tyrosine kinase inhibitor compds.)

RN 317826-08-7 HCAPLUS
CN 2-Pyrimidinamine, N-[(1S)-1-phenylethyl]-4-[5-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1H-benzimidazol-1-yl]- (9CI) (CA INDEX NAME)

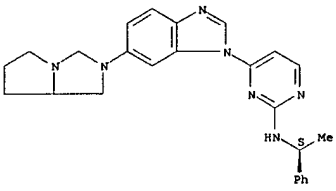
Absolute stereochemistry.

L69 ANSWER 19 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 317826-09-8 HCAPLUS
CN 2-Pyrimidinamine, N-[(1S)-1-phenylethyl]-4-[6-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1H-benzimidazol-1-yl]- (9CI) (CA INDEX NAME)

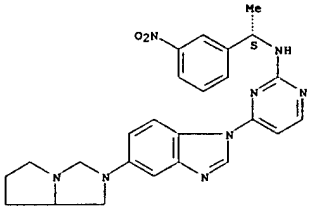
Absolute stereochemistry.



RN 317826-42-9 HCAPLUS
CN 2-Pyrimidinamine, N-[(1S)-1-(3-nitrophenyl)ethyl]-4-[5-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1H-benzimidazol-1-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L69 ANSWER 19 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L69 ANSWER 20 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:12267 HCAPLUS
DOCUMENT NUMBER: 134:71602
TITLE: Preparation and effect of benzimidazolylpyrimidine derivatives as SRC kinase inhibitors
INVENTOR(S): Goulet, Joung L.; Holmes, Mark A.; Hunt, Julianne A.; Mills, Sander G.; Parsons, William H.; Sinclair, Peter J.; Zaller, Dennis M.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 173 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000207	A1	20010104	WO 2000-US17510	20000626
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2376957	AA	20010104	CA 2000-2376957	20000626
US 6329380	B1	20011211	US 2000-603688	20000626
EP 1206260	A1	20020522	EP 2000-953637	20000626
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003503351	T2	20030128	JP 2001-505916	20000626

PRIORITY APPLN. INFO.: US 1999-141630P P 19990630
WO 2000-US17510 W 20000626

OTHER SOURCE(S): MARPAT 134:71602
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

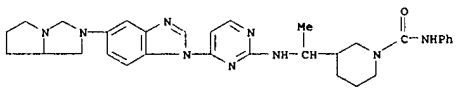
AB Title Pyrimidine compds. [I; R1, R2 independently = H, Br, Cl, I, F, OH, SH, CN, NO2, NH2; R1R2 ; fused methylenedioxy ring, fused 6-membered aromatic ring; R3, R5 independently = H, alkyl, aryl; R3R5 = O; R4 = H, alkyl, alkoxyl; X1, X2, X3, X4 independently = CH, CBr, COH, CSH, CNO2, N; R7 = H, NH2, alkyl, aryl, alkylamino, arylamino; Y = O, N, CH; Z = CO, SO2, bond; m, n independently = 0, 1, 2, 3, 4], or their pharmaceutically acceptable salts, hydrates, solvates, crystal forms and individual diastereomers, and pharmaceutical compns. including the same, which are inhibitors of tyrosine kinase enzymes, and as such are useful in the prophylaxis and treatment of protein tyrosine kinase-associated disorders, such as immune diseases, hyperproliferative disorders and other diseases

L69 ANSWER 20 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

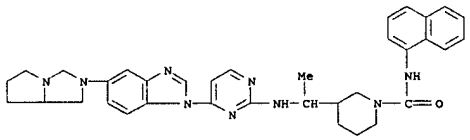
in which inappropriate protein kinase action is believed to play a role, such as cancer, angiogenesis, atherosclerosis, graft rejection, rheumatoid arthritis and psoriasis. Thus, the title compd. II was prepd. and tested.

IT **315717-68-1P 315717-69-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and effect of benzimidazolylpyrimidine derivs. as SRC kinase inhibitors)

RN 315717-68-1 HCAPLUS
CN 1-Piperidinecarboxamide, N-phenyl-3-[1-[[4-[5-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1H-benzimidazol-1-yl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)



RN 315717-69-2 HCAPLUS
CN 1-Piperidinecarboxamide, N-1-naphthalenyl-3-[1-[[4-[5-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1H-benzimidazol-1-yl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)



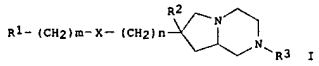
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L69 ANSWER 21 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:139147 HCAPLUS
DOCUMENT NUMBER: 132:175858
TITLE: Drugs containing pyrrolo[1,2-a]pyrazine derivatives as ligands for 5HT1A receptor and imaging of the organs using the derivatives
INVENTOR(S): Sannar, Mark A.
PATENT ASSIGNEE(S): Pfizer Products Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

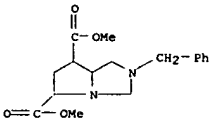
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000063276	A2	20000229	JP 1999-230267	19990817
JP 3356726	B2	20021216		
US 6284757	B1	20010904	US 1999-372438	19990811
CA 2280447	AA	20000217	CA 1999-2280447	19990813
CA 2280447	C	20050329		
MX 9907598	A	20000331	MX 1999-7598	19990817
BR 9906169	A	20000815	BR 1999-6169	19990817
PRIORITY APPLN. INFO.:			US 1998-96875P P	19980817

OTHER SOURCE(S): MARPAT 132:175858
GI



AB The derivs. I [R1 = Ph, naphthyl, benzoxazolonyl, indolyl, indolonyl, benzimidazolinyl, quinolyl, furyl, benzofuryl, thienyl, benzothienyl, oxazolinyl, benzoxazolyl; R2 = H, C1-6 alkyl; R3 = Ph, pyridinyl, pyrimidinyl, pyrazinyl, pyridazinyl; R4, R5 = H, C1-6 alkyl; R1-R3 may be substituted with 1-4 F, C, Br, iodo, cyano, NO2, thiocyano, SR4, SOR4, SO2R4, NHSOR4, C1-6 alkoxy, NR4R5, NR4COR5, CONR4R5, Ph, COR4, CO2R4, C1-6 (halo)alkyl, C3-6 cycloalkyl, OCF3; X = O, S, SO, SO2, NR4, CO, CH(OH), CHR4, OCO, CO2, NR4CO, CONR4; m = 0, 1; n = 0, 1, 2] or their pharmaceutically acceptable salts enhance or inhibit serotonergic neurotransmission, and are useful for treatment of diseases, e.g. headache, anxiety, depression, post-traumatic stress disorders, neurodegenerative disorders, prostatic cancer, drug addictions, etc. Also claimed are imaging of organs using I labeled with radioisotopes or by combination of I with radiomimetic agents, and compns. for the imaging. I are also ligands of dopamine D4 receptor and useful for treatment of

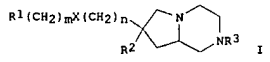
L69 ANSWER 21 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
diseases through enhancing or suppressing dopaminergic neurotransmission.
IT 193068-03-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrrolo[1,2-a]pyrazine derivs. as ligands for 5HT1A receptor)
RN 193068-03-0 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-5,7-dicarboxylic acid, hexahydro-2-(phenylmethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



L69 ANSWER 22 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:98051 HCAPLUS
DOCUMENT NUMBER: 128:154101
TITLE: Preparation of 2,7-disubstituted octahydropyrrolo[1,2-a]pyrazine derivatives as dopamine D4 receptor ligands.
INVENTOR(S): Sanner, Mark A.
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: U.S., 26 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

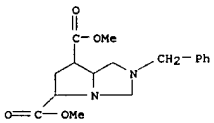
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5714487	A	19980203	US 1996-774290	19961223
PRIORITY APPLN. INFO.:			US 1996-774290	19961223

OTHER SOURCE(S): MARPAT 128:154101
GI



AB Title compds. [I; R1 = Ph, naphthyl, benzoxazolonyl, indolyl, indolonyl, benzimidazolyl, quinolyl, furyl, benzofuryl, thienyl, benzothienyl, oxazolyl, benzoxazolyl; R2, R4 = H, alkyl; R3 = Ph, pyridyl, pyrimidinyl, pyrazinyl, pyridazinyl; m, n = 0-2; X = O, S, SO, SO2, NR4, CO, CHOH, CO2, CHR4, CONR4, etc.], were prepared Thus, (7RS,8aSR)-7-(4-fluorophenoxy)methyl-2-phenylmethyl-1,2,3,4,6,7,8,8a-octahydropyrrolo[1,2-a]pyrazine (preparation given) was refluxed with ammonium formate and Pd/C in MeOH and the residue was refluxed with 2-chloro-6-fluoropyrimidine and Na2CO3 in H2O to give (7RS,8aSR)-7-(4-fluorophenoxy)methyl-2-(5-fluoropyrimidin-2-yl)-1,2,3,4,6,7,8,8a-octahydropyrrolo[1,2-a]pyrazine. I showed binding affinities for displacement of [3H]-spiperone of <2 μM.
IT 193068-03-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2,7-disubstituted octahydropyrrolo[1,2-a]pyrazine derivs. as dopamine D4 receptor ligands)
RN 193068-03-0 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-5,7-dicarboxylic acid, hexahydro-2-(phenylmethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

L69 ANSWER 22 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

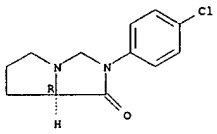


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L69 ANSWER 23 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:753972 HCAPLUS
DOCUMENT NUMBER: 128:123431
TITLE: Inhibition of frog skeletal muscle sodium channels by newly synthesized chiral derivatives of mexiletine and tocainide
AUTHOR(S): De Luca, Annamaria; Natuzzi, Fedele; Falcone, Giulia; Duranti, Andrea; Lentini, Giovanni; Franchini, Carlo; Tortorella, Vincenzo; Conte Camerino, D.
CORPORATE SOURCE: Facolta di Farmacia, Dipartimento Farmacobiologico, Unita di Farmacologia, Via Orabona 4, Bari, I-70125, Italy
SOURCE: Naunyn-Schmiedeberg's Archives of Pharmacology (1997), 356(6), 777-787
CODEN: NSAPCC; ISSN: 0028-1298
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
AB To search for potent use-dependent blockers of skeletal muscle sodium channels as potential antimyotonic agents, the actions of newly synthesized chiral analogs of mexiletine and tocainide were tested in vitro on sodium currents of single fibers of frog semitendinosus muscle by vaseline-gap voltage clamp method. The effect of each drug on the maximal peak Na+ transient (INa max) was evaluated as both tonic and use-dependent block by using infrequent depolarizing stimulation and trains of pulses at 2-10 Hz frequency, resp. The mexiletine analog 3-(2,6-dimethylphenoxy)-2-methylpropanamine (Me2), having an increased distance between the Ph and the amino groups, was less potent than mexiletine in producing a tonic block but produced a remarkable use-dependent block. In fact, the half-maximal concentration (IC50) for tonic block of S(-)-Me2 was 108 μM vs. 54.5 μM of R(-)-mexiletine, but the IC50 was 6.2 times lowered by the 10 Hz stimulation with respect to the 2.4-fold decrease observed with mexiletine. The R(-)-mexiletine and the S(-)-Me2 were about twofold more potent than the corresponding enantiomers in producing a tonic block, but the stereoselectivity attenuated during use-dependent blockade. The more lipophilic 2-(4-chloro-2-methylphenoxy)-1-phenylethylamine (Me1), presently available as raceme, produced a potent and irreversible tonic block of the sodium currents with an IC50 of 29 μM, but had a less pronounced use-dependent inhibition, with a 1.9-fold decrease of the IC50 at 10 Hz. The R(-) isomer of 2',6'-valinoxylidide (To1), a tocainide derivative with an increased hindrance on the chiral carbon atom, was twofold (IC50 = 209 μM) and tenfold (IC50 = 27.4 μM) more potent than R(-)-tocainide in tonic and use-dependent block, resp. Tocainide was almost devoid of stereoselectivity, whereas the eudismic ratio of To1 [IC50 S(+)-To1/IC50 R(-)-To1] was 1.7. As for mexiletine and Me2, the stereoselectivity of To1 was the weaker the higher the frequency of stimulation. The cyclic pyrroloimidazolonic tocainide analog To2 produced

L69 ANSWER 23 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
a small tonic block at 500 μM, and 1 min stimulation at 10 Hz was needed to show up a 50 block of INa max. All the compds. produced a left-shift of the steady-state inactivation curve correlated pos. with the extent of use-dependent inhibition, with the exception of the cyclic To2 that acted as an open-channel blocker. The highly use-dependent blockers Me2 and To1 might be promising drugs to solve high frequency discharges of action potentials typical of myotonic muscles. Concomitantly the high potency of Me1 and the open-channel block exerted by To2 can represent important features to get selective blockers for skeletal muscle sodium channels.
IT 201986-87-0 201986-88-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(inhibition of frog skeletal muscle sodium channels by newly synthesized chiral derivs. of mexiletine and tocainide)
RN 201986-87-0 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-chlorophenyl)hexahydro-, monohydrobromide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

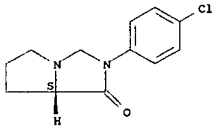


● HBr

RN 201986-88-1 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-chlorophenyl)hexahydro-, monohydrobromide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

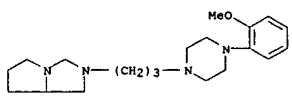
L69 ANSWER 23 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● HBr

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

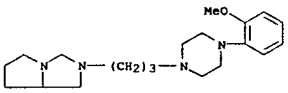
L69 ANSWER 24 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:528590 HCAPLUS
DOCUMENT NUMBER: 127:130461
TITLE: Synthesis and Structure-Activity Relationships of a New Model of Arylpiperazines. 3. 2-[ω-(4-Arylpiperazin-1-yl)alkyl]perhydropyrrolo[1,2-c]imidazol s and -perhydroimidazo[1,5-a]pyridines: Study of the Influence of the Terminal Amide Fragment on 5-HT1A Affinity/Selectivity
AUTHOR(S): Lopez-Rodriguez, Maria L.; Morcillo, M. Jose; Fernandez, Esther; Porras, Esther; Murcia, Marta; Sanz, Antonio M.; Orensanz, Luis
CORPORATE SOURCE: Departamento de Quimica Organica I Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, 28040, Spain
SOURCE: Journal of Medicinal Chemistry (1997), 40(16), 2653-2656
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of new arylpiperazine derivs., which are devoid of the terminal amide fragment present in related 5-HT1A ligands, was prepared and evaluated for affinity at 5-HT1A and α1 receptors. All the compds. demonstrated high affinity for the 5-HT1A receptor and moderate affinity for α1 receptor binding sites. Structure-activity relationship (SAR) studies suggest that there is influence of electronic factors on the no-pharmacophoric part of the α1 receptor site. However there is no influence of electronic interactions on the stabilization of the 5-HT1A receptor-ligand complex.
IT 192993-08-1P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(preparation and affinity at α1- and 5-HT1A-receptors of arylpiperazines)
RN 192993-08-1 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole, hexahydro-2-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-, tetrahydrochloride (9CI) (CA INDEX NAME)



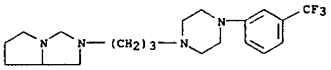
●4 HCl

IT 192992-82-8P 192992-83-9P 192992-86-2P 192992-87-3P 192992-88-4P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN

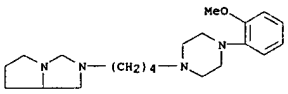
L69 ANSWER 24 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(prepn. and affinity at α1- and 5-HT1A-receptors of arylpiperazines)
RN 192992-82-8 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole, hexahydro-2-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)



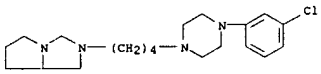
RN 192992-83-9 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole, hexahydro-2-[3-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)



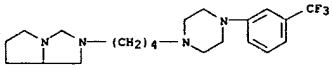
RN 192992-86-2 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole, hexahydro-2-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



RN 192992-87-3 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole, 2-[4-[4-(3-chlorophenyl)-1-piperazinyl]butyl]hexahydro- (9CI) (CA INDEX NAME)



L69 ANSWER 24 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 192992-88-4 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole, hexahydro-2-[4-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



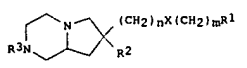
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L69 ANSWER 25 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:506300 HCAPLUS
DOCUMENT NUMBER: 127:135811
TITLE: Preparation of 2,7-substituted octahydropyrrolo[1,2-a]pyrazine derivatives as ligands for dopamine receptor subtypes
INVENTOR(S): Sanner, Mark A.
PATENT ASSIGNEE(S): Pfizer Inc., USA; Sanner, Mark A.
SOURCE: PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9723482	A1	19970703	WO 1996-IB1192	19961106
W: AU, BG, BR, BY, CA, CN, CZ, HU, IL, IS, JP, KR, KZ, LK, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2240594	AA	19970703	CA 1996-2240594	19961106
CA 2240594	C	20010724		
AU 9673280	A1	19970717	AU 1996-73280	19961106
AU 704578	B2	19990429		
EP 874849	A1	19981104	EP 1996-935226	19961106
EP 874849	B1	20010919		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LV, FI, RO				
CN 1205704	A	19990120	CN 1996-199250	19961106
CN 1061350	B	20010131		
BR 9612246	A	19990713	BR 1996-12246	19961106
JP 11508920	T2	19990803	JP 1997-523446	19961106
JP 3204456	B2	20010904		
RU 2162470	C2	20010127	RU 1998-111742	19961106
AT 205846	E	20011015	AT 1996-935226	19961106
ES 2161377	T3	20011201	ES 1996-935226	19961106
PT 874849	T	20020130	PT 1996-935226	19961106
TW 479058	B	20020311	TW 1996-85113669	19961108
ZA 9610781	A	19980622	ZA 1996-10781	19961220
NO 9802843	A	19980619	NO 1998-2843	19980619
NO 309936	B1	20010423		
GR 3037060	T3	20020131	GR 2001-401932	20011030

PRIORITY APPLN. INFO.: US 1995-8988P P 19951221
WO 1996-IB1192 W 19961106

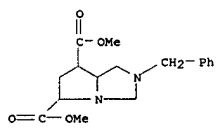
OTHER SOURCE(S): MARPAT 127:135811
GI



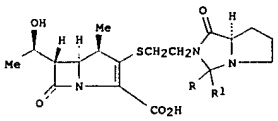
I

AB I [R1 = Ph, naphthyl, benzoxazolonyl, indolyl, indolonyl, benzimidazolyl,

L69 ANSWER 25 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
quinolyl, furyl, benzofuryl, thienyl, benzothienyl, oxazolyl, benzoxazolyl; R2 = H, (C1-C6)alkyl; R3 = Ph, pyridinyl, pyrimidinyl, pyrazinyl, pyridazinyl; X = O, S, SO, SO2, NR4, CO, CH(OH), CHR4, etc.; m = 0, 1, 2; n = 0, 1, 2] were prepd as ligands for dopamine receptor subtypes, esp. the dopamine D4 receptor. E.g., (7RS,8aSR)-7-(4-fluorophenoxy)-2-phenylmethyl-1,2,3,4,6,7,8,8a-octahydropyrrolo[1,2-a]pyrazine and aq. ammonium formate in MeOH was treated with an aq. slurry
of 10% Pd/C and the product then reacted with 2-chloro-5-fluoropyrimidine to give (7RS,8aSR)-7-(4-fluorophenoxy)-2-(5-fluoropyrimidin-2-yl)-1,2,3,4,6,7,8,8a-octahydropyrrolo[1,2-a]pyrazine. The title compds. had D4 binding affinities for the displacement of [3H]-spiperone < 2 micromolar.
IT 193068-03-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2,7-substituted octahydropyrrolo[1,2-a]pyrazine derivs. as
ligands for D4 dopamine receptors)
RN 193068-03-0 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-5,7-dicarboxylic acid, hexahydro-2-(phenylmethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



L69 ANSWER 26 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:701300 HCAPLUS
DOCUMENT NUMBER: 126:89181
TITLE: Synthesis and antibacterial activity of 1-β-methylcarbapenems having a 1,3-diazabicyclo[3.3.0]octan-4-one moiety
AUTHOR(S): Nam, Ki Hong; Oh, Chang Hyun; Cho, Jin Koo; Kim, Hyo Jung; Lee, Ki Soo; Cho, Jung Hyuck
CORPORATE SOURCE: Division Applied Science, Korea Institute Science Technology, Seoul, 130-650, S. Korea
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1996), 329(10), 443-446
CODEN: ARPMAS; ISSN: 0365-6233
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

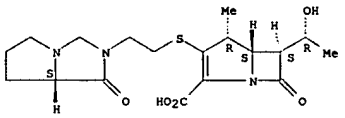
AB The synthesis of the methylcarbapenems I (R, R1 = H; R = Me; R1 = H, Me, Et, Pr, Ph or R = cyclopropyl; R1 = H, Me) from protected 2-(diphenylphosphoryloxy)carbapenem and the appropriate mercaptoethyldiazabicyclooctanone is described. Their in-vitro antibacterial activities against both Gram-pos. and Gram-neg. bacteria are reported. The effect of the substituent on the bicyclic ring was investigated in agreement with findings from our previous studies.

IT **185736-63-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antibacterial activity of diazabicyclooctanone-substituted carbapenems)

RN 185736-63-4 HCAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-(1-hydroxyethyl)-4-methyl-7-oxo-3-[[2-(tetrahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)ethyl]thio]-, [4R-[3(S*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

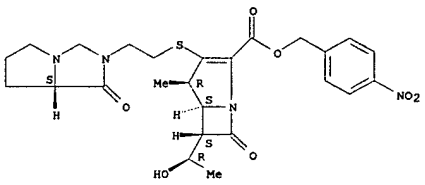
L69 ANSWER 26 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT **185736-80-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and antibacterial activity of diazabicyclooctanone-substituted carbapenems)

RN 185736-80-5 HCAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-(1-hydroxyethyl)-4-methyl-7-oxo-3-[[2-(tetrahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)ethyl]thio]-, (4-nitrophenyl)methyl ester, [4R-[3(S*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

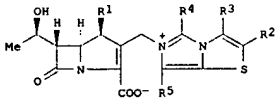
Absolute stereochemistry.



L69 ANSWER 27 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:674366 HCAPLUS
DOCUMENT NUMBER: 125:328383
TITLE: Preparation of novel carbapenem derivatives as antibacterials
INVENTOR(S): Aihara, Kazuhiro; Kano, Yuko; Shiokawa, Sohjiro; Sasaki, Toshiro; Setsu, Fumihito; Toyooka, Yumiko; Ishii, Miyuki; Atsumi, Kunio; Iwamatsu, Katsuyoshi; Tamura, Atsushi
PATENT ASSIGNEE(S): Meiji Seika Kabushiki Kaisha, Japan
SOURCE: PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9628455	A1	19960919	WO 1996-JP573	19960308
W: CA, CN, CZ, HU, JP, KR, PL, SI, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2189995	AA	19960919	CA 1996-2189995	19960308
CA 2189995	C	20010123		
EP 760370	A1	19970305	EP 1996-905036	19960308
EP 760370	B1	20020807		
R: BE, DE, ES, FR, GB, IT, NL				
CN 1148390	A	19970423	CN 1996-190177	19960308
CN 1057091	B	20001004		
ES 2179932	T3	20030201	ES 1996-905036	19960308
TW 425396	B	20010311	TW 1996-85102872	19960309
US 5990101	A	19991123	US 1997-737232	19970312
PRIORITY APPLN. INFO.:			JP 1995-51616 A	19950310
			WO 1996-JP573 W	19960308

OTHER SOURCE(S): MARPAT 125:328383
GI



I

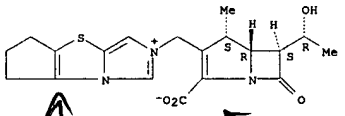
AB Title compds. I [R1 = H, alkyl; R2-R5 = H, halo, OH, nitro, cyano, COOH, formyl, alkyl, cycloalkyl, C2-4 alkenyl, C2-4 alkynyl, alkoxy, etc.] are prepared The compds. have a broad and potent antibacterial activity on Gram-pos. bacteria and Gram-neg. bacteria including Pseudomonas aeruginosa and show a potent antibacterial effect on various β-lactamase-producing bacteria and MRSA and an extremely high DHP-1 stability. Thus,

L69 ANSWER 27 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
allyl (1S,5R,6S)-6-[(1R)-1-(allyloxycarbonyloxy)ethyl]-2-(hydroxymethyl)-1-methyl-1-carbapen-2-em-2-carboxylate was reacted with di-Ph phosphorochloridate in CH2Cl2 contg. 4-(dimethylamino)pyridine to give the corresponding phosphate, which was reacted with 3-(hydroxymethyl)imidazo[5,1-b]thiazole in DMF contg. NaI, and the product treated with Ph3P, 2-ethylhexanoic acid, potassium 2-ethylhexanoate, and tetrakis(triphenylphosphine)palladium in CH2Cl2 at room temp. for 2 h to give the title compd. I [R1 = Me, R2 = CH2OH, R3-R5 = H]. This had an MIC comparable to that of imipenem/cilastatin against Staphylococcus aureus. Pharmaceutical compns. contg. I are described.

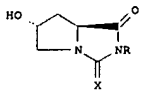
IT **183067-38-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel carbapenem derivs. as antibacterials)

RN 183067-38-1 HCAPLUS
CN 5H-Cyclopent[d]imidazo[5,1-b]thiazolium, 2-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]methyl]-6,7-dihydro-, inner salt, [4S-[4α,5β,6β(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



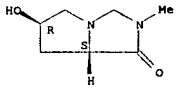
L69 ANSWER 28 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:1000583 HCAPLUS
DOCUMENT NUMBER: 124:175947
TITLE: An efficient construction of 4-oxo-1,3-diazabicyclo[3.3.0]octanes via thiohydantoins
AUTHOR(S): Kim, In Jong; Yoo, Kyung Ho; Shin, Kye Jung; Kim, Dong Jin; Park, Sang Woo
CORPORATE SOURCE: Div. Applied Science, Korea Inst. Science Technology, Seoul, 131-650, S. Korea
SOURCE: Synthetic Communications (1995), 25(24), 4001-10
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Dekker
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:175947
GI



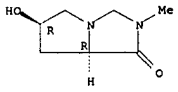
I

AB New stereoisomeric N-bridged heterocycles, 4-oxo-1,3-diazabicyclo[3.3.0]octanes (I; R = Me, Et, Ph, 4-MeC6H4, X = H,H) were synthesized from trans-4-hydroxy-L-proline (II). Thiohydantoins I (X = S) as the key intermediates were prepared by nucleophilic addition of II to isothiocyanates, and subsequent cyclization. These thiohydantoins I (X = S) were readily desulfuriized to provide I (X = H,H).
IT **173549-72-9P 173549-73-0P 173549-74-1P**
173549-75-2P 173658-16-7P 173658-17-8P
173658-18-9P 173658-19-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(efficient preparation of oxodiazabicyclooctanes from hydroxyproline via thiohydantoins)
RN 173549-72-9 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-6-hydroxy-2-methyl-, (6R-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

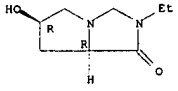


L69 ANSWER 28 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



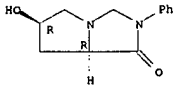
RN 173658-17-8 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-ethylhexahydro-6-hydroxy-, (6R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



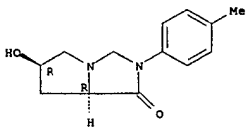
RN 173658-18-9 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-6-hydroxy-2-phenyl-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



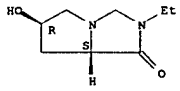
RN 173658-19-0 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-6-hydroxy-2-(4-methylphenyl)-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



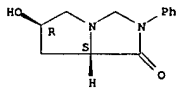
L69 ANSWER 28 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 173549-73-0 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-ethylhexahydro-6-hydroxy-, (6R-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



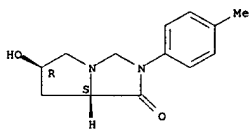
RN 173549-74-1 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-6-hydroxy-2-phenyl-, (6R,7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 173549-75-2 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-6-hydroxy-2-(4-methylphenyl)-, (6R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



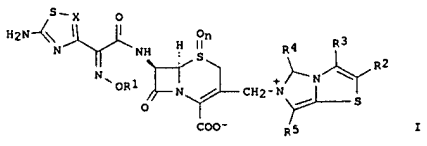
RN 173658-16-7 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-6-hydroxy-2-methyl-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L69 ANSWER 29 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:713780 HCAPLUS
DOCUMENT NUMBER: 123:111745
TITLE: Preparation of antibacterial cephem derivatives
INVENTOR(S): Atsumi, Kunio; Umemura, Eijiro; Kano, Yuko; Shiokawa, Sohjiro; Kudo, Toshiaki; Tsushima, Masaki; Iwamatsu, Katsuyoshi; Tamura, Atsushi; Shibahara, Seiji
PATENT ASSIGNEE(S): Meiji Seika K. K., Japan
SOURCE: PCT Int. Appl., 326 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9507912	A1	19950323	WO 1994-JP1529	19940916
W: CA, CN, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 669336	A1	19950830	EP 1994-927055	19940916
EP 669336	B1	20000517		
R: AT, BE, CH, DE, ES, FR, GB, IE, IT, LI, NL				
CN 1114507	A	19960103	CN 1994-190696	19940916
CN 1046286	B	19991110		
TW 385312	B	20000321	TW 1994-83108591	19940916
AT 192927	E	20000615	AT 1994-927055	19940916
ES 2146661	T3	20000816	ES 1994-927055	19940916
CA 2149514	C	20001031	CA 1994-2149514	19940916
JP 3152934	B2	20010403	JP 1995-509092	19940916
US 5663162	A	19970902	US 1995-436280	19950725
PRIORITY APPLN. INFO.:			JP 1993-230573 A	19930916
			JP 1994-211908 A	19940812
			WO 1994-JP1529 W	19940916

OTHER SOURCE(S): MARPAT 123:111745
GI



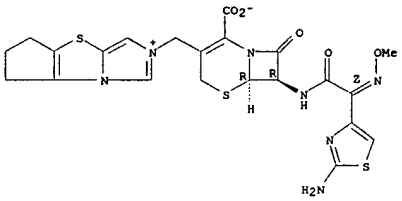
I

AB Title compds. I [R1 represents H, alkyl, alkenyl, etc.; and R2, R3, R4 and R5 represent each H, alkyl, carbamoyl, amino, etc.; n = 0, 1; X = CH, N] are prepared Thus, a mixture of
-ritylaminothiazol-4-yl)-

L69 ANSWER 29 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
2-methoxyimino]acetamido-3-(chloromethyl)-3-cephem-4-carboxylic acid p-methoxybenzyl ester was reacted with imidazo[5,1-b]thiazole (prepn. given) in acetone contg. NaI at room temp. overnight to give, after hydrolysis, (6R,7R)-7-[(Z)-2-(2-aminothiazol-4-yl)-2-

methoxyiminoacetamido]-3-(imidazo[5,1-b]thiazolium-6-ylmethyl)-3-cephem-4-carboxylate inner salt. (6R,7R)-7-(Z)-2-(2-aminothiazol-4-yl)-2-[(S)-1-carboxyethoxyiminoacetamido]-3-(imidazo[5,1-b]thiazolium-6-ylmethyl)-3-cephem-4-carboxylate (also prepd.) had an MIC of 6.25 μg/mL against Staphylococcus aureus. Pharmaceutical compns. contg. I are described.
IT 165665-19-0P 165665-20-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of antibacterial cephem derivs.)
RN 165665-19-0 HCAPLUS
CN 5H-Cyclopent[d]imidazo[5,1-b]thiazolium, 2-[[7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-6,7-dihydro-, inner salt, [6R-[6α,7β(Z)]]- (9CI) (CA INDEX NAME)

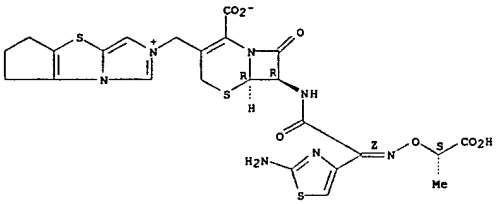
Absolute stereochemistry.
Double bond geometry as shown.



RN 165665-20-3 HCAPLUS
CN 5H-Cyclopent[d]imidazo[5,1-b]thiazolium, 2-[[7-[[(2-amino-4-thiazolyl)[(1-carboxyethoxy)imino]acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-6,7-dihydro-, inner salt, [6R-[6α,7β[Z(S*)]]]- (9CI) (CA INDEX NAME)

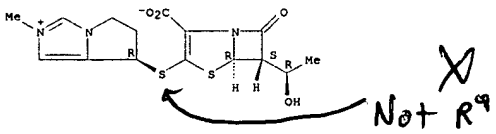
Absolute stereochemistry.
Double bond geometry as shown.

L69 ANSWER 29 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



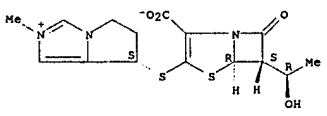
L69 ANSWER 30 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:579312 HCAPLUS
DOCUMENT NUMBER: 121:179312
TITLE: Synthesis and antibacterial activity of new 2-substituted penems. II
AUTHOR(S): Nishi, Toshiyuki; Higashi, Kunio; Soga, Tsunehiko; Takemura, Makoto; Sato, Makoto
CORPORATE SOURCE: Explorat. Res. Lab. I, Daiichi Pharm. Co., Ltd., Tokyo, 134, Japan
SOURCE: Journal of Antibiotics (1994), 47(3), 357-69
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 'A series of new penems, having a bicyclic imidazole moiety as the C-2 substituent, has been synthesized. The antimicrobial activity of these compds. and their susceptibility to renal dehydropeptidase-I are elucidated, and their structure-activity relationships are discussed.
IT 108308-24-3P 108308-25-4P 108309-32-6P
108309-33-7P 118776-90-2P 118776-91-3P
157683-42-6P 157683-43-7P 157683-50-6P
157683-51-7P 157683-52-8P 157683-53-9P
157683-54-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)
RN 108308-24-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-25-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

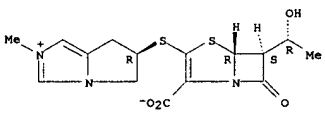
Absolute stereochemistry.



L69 ANSWER 30 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

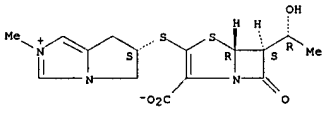
RN 108309-32-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



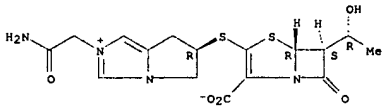
RN 108309-33-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 118776-90-2 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-6-[[(5R,6S)-2-carboxy-6-[(1R)-1-hydroxyethyl]-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-, inner salt (9CI) (CA INDEX NAME)

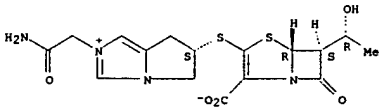
Absolute stereochemistry.



RN 118776-91-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]methyl]-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

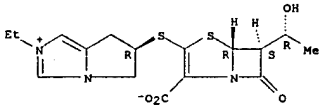
Absolute stereochemistry.

L69 ANSWER 30 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



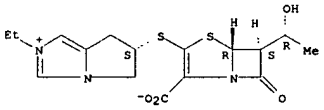
RN 157683-42-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-ethyl-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 157683-43-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-ethyl-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

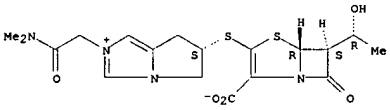
Absolute stereochemistry.



RN 157683-50-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[2-(methylamino)-2-oxoethyl]-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

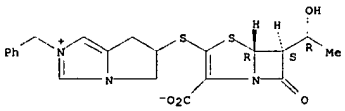
Absolute stereochemistry.

L69 ANSWER 30 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

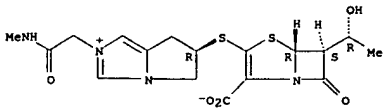


RN 157683-54-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(phenylmethyl)-, inner salt, [5R-[5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

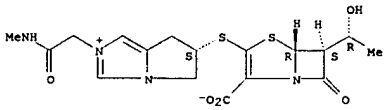


L69 ANSWER 30 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



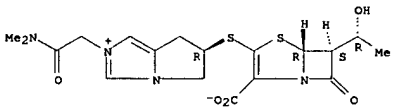
RN 157683-51-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[2-(methylamino)-2-oxoethyl]-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 157683-52-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-[2-(dimethylamino)-2-oxoethyl]-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

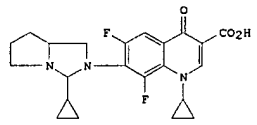


RN 157683-53-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-[2-(dimethylamino)-2-oxoethyl]-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

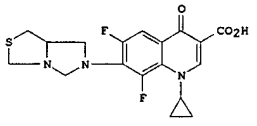
Absolute stereochemistry.

L69 ANSWER 31 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:483169 HCAPLUS
DOCUMENT NUMBER: 121:83169
TITLE: Synthesis of new quinolinone antibacterial agents with diazolidine heterocyclic amines
AUTHOR(S): Cho, Seong Hwan; Cho, H Hwan; Shin, Young Jun; An, Seung Ho
CORPORATE SOURCE: Res. Dev. Cent., Cheil Foods and Chem. Inc., Kyongi, 467-810, S. Korea
SOURCE: Korean Journal of Medicinal Chemistry (1993), 3(2), 162-7
CODEN: KJMCE7; ISSN: 1225-0058
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



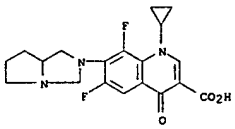
II

AB The title compds., e.g., I and II, were prepared by reaction of 7-haloquinolinones with heterocycles. The antibacterial activity of the products was lower than that of ciprofloxacin.

IT **156171-70-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 156171-70-9 HCAPLUS
CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo-7-(tetrahydro-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)- (9CI) (CA INDEX NAME)

L69 ANSWER 31 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



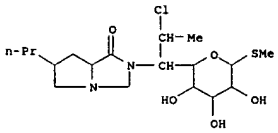
L69 ANSWER 32 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:116630 HCAPLUS
DOCUMENT NUMBER: 120:116630
TITLE: 1H- and 13C-NMR studies of aminoglycoside antibiotics
AUTHOR(S): Moloney, Gerard P.; Craik, David J.; Iskander, Magdy N.
CORPORATE SOURCE: Victorian Coll. Pharm., Monash Univ., Parkville, 3052, Australia
SOURCE: Magnetic Resonance in Chemistry (1993), 31(12), 1077-84
CODEN: MRCHEG; ISSN: 0749-1581
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 1H-NMR spectroscopy was used to determine the conformations of the aminoglycoside antibiotic N-demethylclindamycin and 2 of its cyclic derivs. The conformational features of these systems were determined by consideration of vicinal coupling consts. and, in some cases, Nuclear Overhauser enhancement (NOE) effects. 1H- and 13C-NMR chemical shifts are reported and compared with previous results for the related antibiotic lincomycin. The stability of the 2 cyclized derivs. in aqueous solns. was examined Both cyclizations involved formation of a 4-imidazolidinone ring. The ring system based on cyclization with formaldehyde was stable in aqueous solution, whereas that based on benzaldehyde was not.

IT **35119-67-6**
RL: PRP (Properties)
(conformation of, proton and carbon-13 NMR study of, stability in relation to)

RN 35119-67-6 HCAPLUS
CN L-threo-α-D-galacto-Octopyranoside, methyl 7-chloro-6,7,8-trideoxy-6-(tetrahydro-1-oxo-6-propyl-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1-thio-, (6R-cis)- (9CI) (CA INDEX NAME)



L69 ANSWER 33 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:407730 HCAPLUS
DOCUMENT NUMBER: 117:7730
TITLE: Preparation of carbapenem derivatives
INVENTOR(S): Suzaki, Hiroshi; Nishi, Toshiyuki; Takemura, Makoto; Hayano, Takeshi
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04009380	A2	19920114	JP 1990-109307	19900425
JP 3045518	B2	20000529		
PRIORITY APPLN. INFO.:			JP 1990-109307	19900425

OTHER SOURCE(S): MARPAT 117:7730
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Carbapenem derivs. [I; R1 = alkyl, (protected) hydroxyalkyl; R2 = H, protecting group, anion; R3 = H, alkyl; R4 = (substituted) fused heterocyclyl containing ≥2 N atoms and an onium center], useful as antibacterial agents, are prepared MeI was added to a solution of 165 mg ester II in Me2CO with stirring at 5°, more MeI was added, and the mixture was stirred at 5° and the distillate residue was dissolved in phosphate buffer and hydrogenolyzed over 10% Pd-C at 4 atm H to give 23 mg (1R,5S,6S,8R)-III (IV) and 18 mg isomer. IV showed MIC of <0.1 μg/mL against Escherichia coli NIHJ, etc.

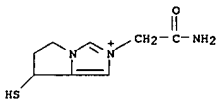
IT **118776-50-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antibacterial agent)

RN 118776-50-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-6,7-dihydro-7-mercapto-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 118776-49-1
CMF C8 H12 N3 O S

L69 ANSWER 33 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



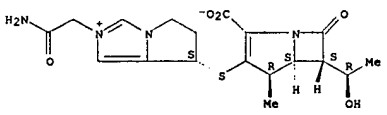
CM 2

CRN 37181-39-8
CMF C F3 O3 S

IT **141547-45-7P 141547-46-8P 141547-47-9P**
141611-04-3P 141611-05-4P 141611-06-5P
141611-07-6P 141611-08-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibacterial agent)

RN 141547-45-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-7-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-, inner salt, [4R-[3(S*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

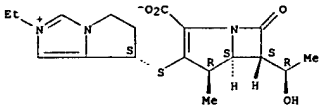
Absolute stereochemistry.



RN 141547-46-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-ethyl-6,7-dihydro-, inner salt, [4R-[3(S*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

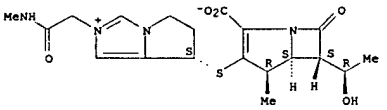
L69 ANSWER 33 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 141547-47-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium,
7-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-

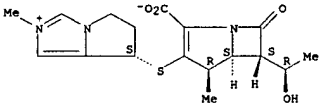
oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[2-(methylamino)-
2-oxoethyl]-, inner salt, [4R-[3(S*),4α,5β,6β(R*)]]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



RN 141611-04-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium,
7-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-
oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner
salt, [4R-[3(S*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

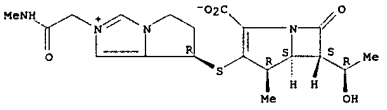
Absolute stereochemistry.



RN 141611-05-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium,
7-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-
oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner
salt, [4R-[3(R*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

L69 ANSWER 33 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

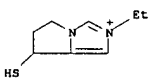
Absolute stereochemistry.



IT **141547-44-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carbapenem derivative, in preparation of
antibacterial agent)
RN 141547-44-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-ethyl-6,7-dihydro-7-mercapto-, salt with
trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

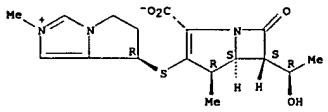
CRN 141547-43-5
CMF C8 H13 N2 S



CM 2

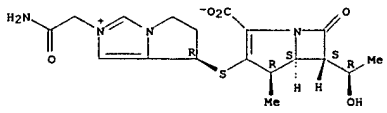
CRN 37181-39-8
CMF C F3 O3 S

L69 ANSWER 33 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.



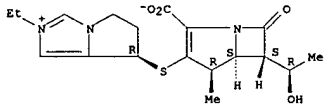
RN 141611-06-5 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-7-[[2-carboxy-6-(1-
hydroxyethyl)-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-
dihydro-, inner salt, [4R-[3(R*),4α,5β,6β(R*)]]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



RN 141611-07-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium,
7-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-
oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-ethyl-6,7-dihydro-, inner
salt, [4R-[3(R*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

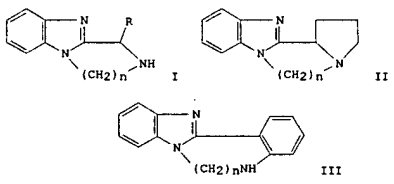
Absolute stereochemistry.



RN 141611-08-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium,
7-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-

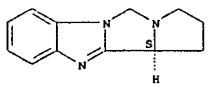
oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[2-(methylamino)-
2-oxoethyl]-, inner salt, [4R-[3(R*),4α,5β,6β(R*)]]- (9CI)
(CA INDEX NAME)

L69 ANSWER 34 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:514421 HCAPLUS
DOCUMENT NUMBER: 115:114421
TITLE: Heterocyclization of the 2-aminoalkyl(and aryl)benzimidazoles under phase transfer catalysis conditions
AUTHOR(S): Cherkaoui, O.; Essassi, E. M.; Zniber, R.
CORPORATE SOURCE: Dep. Chim., Fac. Sci., Rabat, Morocco
SOURCE: Bulletin de la Societe Chimique de France (1991), (March-April), 255-9
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 115:114421
GI



AB New imidazole (pyrazino and diazepino) benzimidazoles, e.g. I (R = H, Me, n = 1,2,3), II (n = 1,2,3), and III (n = 1,2), were prepared by reaction between 2-aminoalkyl (and aryl) benzimidazoles and dibromoalkanes Br(CH2)nBr (n = 1,2,3) under phase transfer catalysis conditions. These products were characterized by 1H-NMR, IR, MS, and microanal.
IT **135875-12-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from o-phenylenediamine, amino acid, and dibromoalkane)
RN 135875-12-6 HCAPLUS
CN 5H-Pyrrolo[1',2':3,4]imidazo[1,5-a]benzimidazole, 1,2,3,11b-tetrahydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



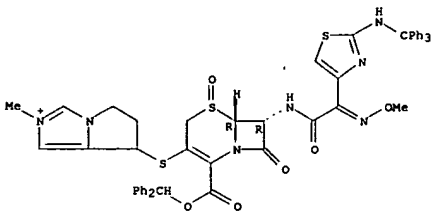
L69 ANSWER 35 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:228624 HCAPLUS
DOCUMENT NUMBER: 114:228624
TITLE: 3-Cephem-4-carboxylic acids as antibiotics
INVENTOR(S): Sasaki, Takashi; Hayano, Takeshi; Takemura, Makoto; Tagawa, Hiroaki
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01272590	A2	19891031	JP 1988-98053	19880422
JP 2568248	B2	19961225		
PRIORITY APPLN. INFO.:			JP 1988-98053	19880422

OTHER SOURCE(S): MARPAT 114:228624
GI For diagram(s), see printed CA Issue.
AB Title compds. I [Y = C,N; R = Cl, R1 = H, protecting group; R2 = H, cyclopropyl-, cyano-, carbamoyl-, or (protected) CO2H-substituted alkyl, Q; R3 = (protected) CO2H, carboxylate; R4 = H, (N-alkyl or N,N-dialkyl)carbamoyl-, cyano-, or (protected) CO2H-substituted alkyl], useful as antibiotics especially for treating drug-resistant bacteria, gram (+)-bacteria, and Pseudomonas aeruginosa, are prepared A diastereomer of I [R = 6,7-dihydro-2-methyl-5H-pyrrolo[1,2-c]imidazolinium-7-yl; R1 = H;R2 = Me; R3 = CO2-] showed MIC's of 12.5, <0.1, and 0.20 μg/mL against P. aeruginosa, Escherichia coli, and Staphylococcus aureus, resp., vs. 25, <0.1, and 3.13 μg/mL for cefotaxime.
IT 127112-06-5P 127112-07-6P 127112-10-1P
127112-13-4P 127112-14-5P 127134-54-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of cephemcarboxylates)
RN 127112-06-5 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-[(diphenylmethoxy)carbonyl]-7-[[(methoxyimino)[2-[(triphenylmethyl)amino]-4-thiazolyl]acetyl]amino]-5-oxido-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, iodide, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

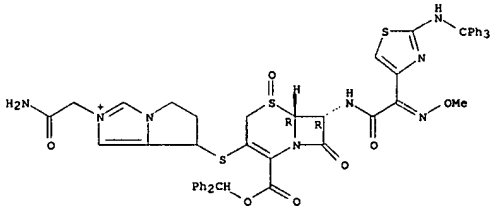
L69 ANSWER 35 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● I⁻

RN 127112-07-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-7-[[2-[(diphenylmethoxy)carbonyl]-7-[[(methoxyimino)[2-[(triphenylmethyl)amino]-4-thiazolyl]acetyl]amino]-5-oxido-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-, iodide, (6R-(6α,7β))- (9CI) (CA INDEX NAME)

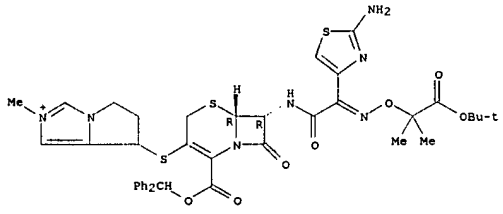
Absolute stereochemistry.
Double bond geometry unknown.



● I⁻

L69 ANSWER 35 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 127112-10-1 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[(2-amino-4-thiazolyl)[[2-(1,1-dimethylethoxy)-1,1-dimethyl-2-oxoethoxy]imino]acetyl]amino]-2-[(diphenylmethoxy)carbonyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, iodide, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

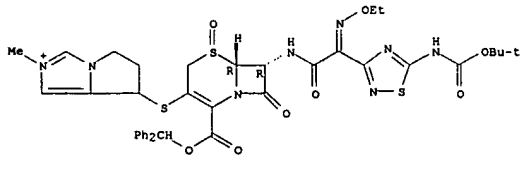
Absolute stereochemistry.
Double bond geometry unknown.



● I⁻

RN 127112-13-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[[5-[[(1,1-dimethylethoxy)carbonyl]amino]-1,2,4-thiadiazol-3-yl](ethoxyimino)acetyl]amino]-2-[(diphenylmethoxy)carbonyl]-5-oxido-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, iodide, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

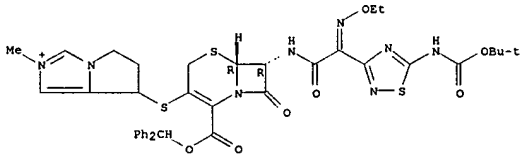


● I⁻

RN 127112-14-5 HCAPLUS

L69 ANSWER 35 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[[5-[[(1,1-dimethylethoxy)carbonyl]amino]-1,2,4-thiadiazol-3-yl](ethoxyimino)acetyl]amino]-2-[(diphenylmethoxy)carbonyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, iodide, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

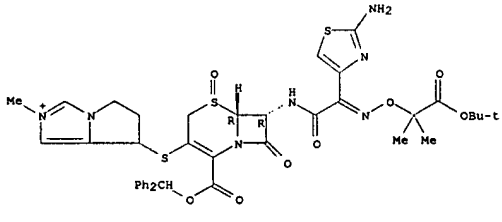
Absolute stereochemistry.



● I⁻

RN 127134-54-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[[2-amino-4-thiazolyl][[2-(1,1-dimethylethoxy)-1,1-dimethyl-2-oxoethoxy]imino]acetyl]amino]-2-[(diphenylmethoxy)carbonyl]-5-oxido-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, iodide, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



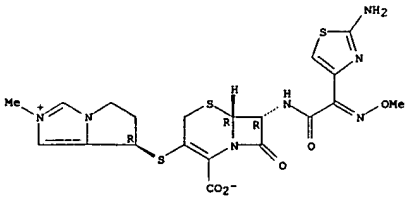
● I⁻

IT 127111-78-8P 127111-79-9P 127111-80-2P

L69 ANSWER 35 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
127111-81-3P 127111-82-4P 127111-85-7P
127111-86-8P 127111-89-1P 127111-90-4P
127111-95-9P 127111-96-0P 127134-53-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of, as antibiotic)

RN 127111-78-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [6R-[3(R*),6α,7β]]- (9CI) (CA INDEX NAME)

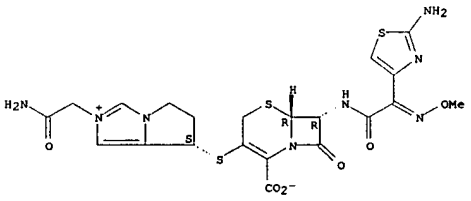
Absolute stereochemistry.
Double bond geometry unknown.



RN 127111-79-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [6R-[3(S*),6α,7β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

L69 ANSWER 35 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 127111-82-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[(2-amino-4-thiazolyl)[(1-carboxy-1-methylethoxy)imino]acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, chloride, monohydrochloride, [6R-[3(R*),6α,7β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

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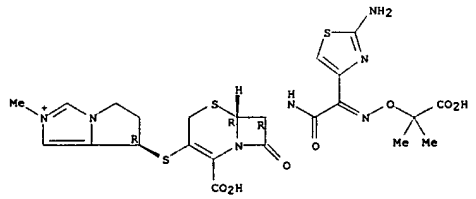


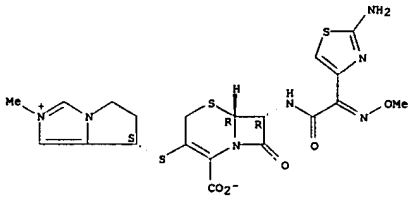
● Cl⁻

PAGE 2-A

● HCl

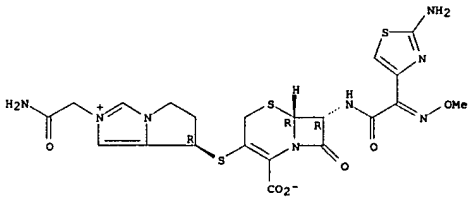
RN 127111-85-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[(5-amino-1,2,4-thiadiazol-3-yl)(ethoxyimino)acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [6R-[3(R*),6α,7β]]- (9CI) (CA INDEX NAME)

L69 ANSWER 35 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 127111-80-2 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-7-[[7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-, inner salt, [6R-[3(R*),6α,7β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

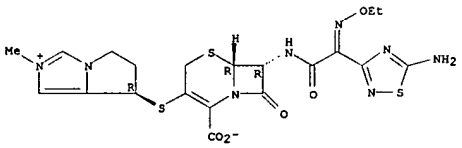


RN 127111-81-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-7-[[7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-, inner salt, [6R-[3(S*),6α,7β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

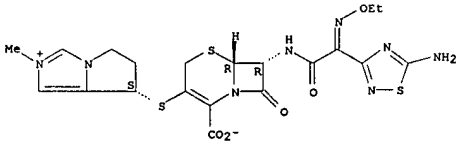
L69 ANSWER 35 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.



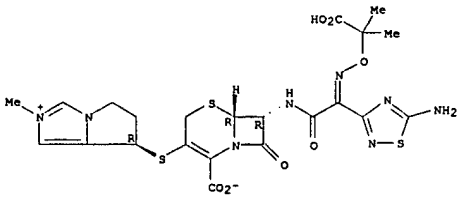
RN 127111-86-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[(5-amino-1,2,4-thiadiazol-3-yl)(ethoxyimino)acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [6R-[3(S*),6α,7β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



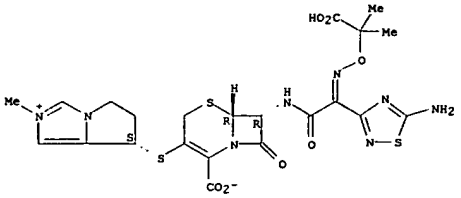
RN 127111-89-1 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[(5-amino-1,2,4-thiadiazol-3-yl)[(1-carboxy-1-methylethoxy)imino]acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [6R-[3(R*),6α,7β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



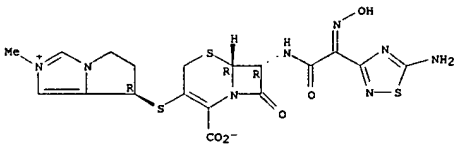
L69 ANSWER 35 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 127111-90-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[(5-amino-1,2,4-thiadiazol-3-yl)[(1-carboxy-1-methylethoxy)imino]acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [6R-[3(S*),6α,7β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 127111-95-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[(5-amino-1,2,4-thiadiazol-3-yl)(hydroxyimino)acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [6R-[3(R*),6α,7β]]- (9CI) (CA INDEX NAME)

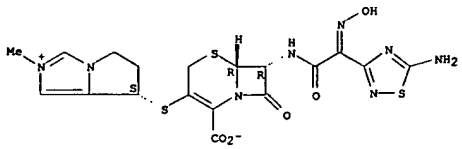
Absolute stereochemistry.



RN 127111-96-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[(5-amino-1,2,4-thiadiazol-3-yl)(hydroxyimino)acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [6R-[3(S*),6α,7β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

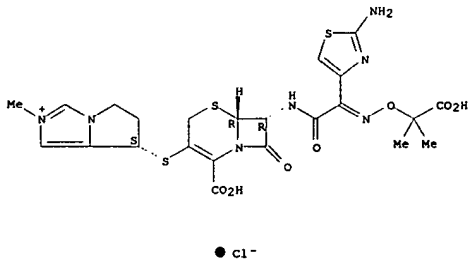
L69 ANSWER 35 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 127134-53-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[7-[[(2-amino-4-thiazolyl)[(1-carboxy-1-methylethoxy)imino]acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, chloride, monohydrochloride, [6R-[3(S*),6α,7β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



● Cl⁻

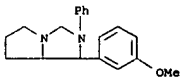
PAGE 2-A

● HCl

L69 ANSWER 36 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:128873 HCAPLUS
DOCUMENT NUMBER: 112:128873
TITLE: Nonlinear optical material
INVENTOR(S): Takeya, Yutaka; Matsuzawa, Hiroshi; Iwata, Kaoru
PATENT ASSIGNEE(S): Teijin Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01245084	A2	19890929	JP 1988-72081	19880328
PRIORITY APPLN. INFO.:			JP 1988-72081	19880328

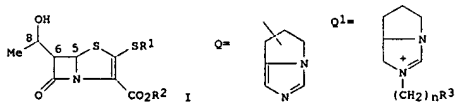
AB A nonlinear optical material, suited for use in optical switches, memories, and bistable devices, consists of a carbonic acid ester represented by RA(CH:CH)nCH:C(CN)CO2L (R = R1R2N, R3O, R4S, CN, CONR5R6, NR7COR8, R9; R1-9 = C1-8 hydrocarbyl, H; A = C5-14 aryl; L = C12-25 straight-chain hydrocarbyl; n = 0, 1, 2).
IT **125811-46-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, nonlinear optical material from)
RN 125811-46-3 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole, hexahydro-1-(3-methoxyphenyl)-2-phenyl- (9CI) (CA INDEX NAME)



L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:75160 HCAPLUS
DOCUMENT NUMBER: 110:75160
TITLE: Preparation of 6-(1-hydroxyethyl)-2-penem-3-carboxylate derivatives as antibacterials
INVENTOR(S): Takemura, Makoto; Azuma, Kunio; Nishi, Toshiyuki; Koda, Hiroko; Sato, Makoto
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63154691	A2	19880627	JP 1986-300810	19861217
JP 2579472	B2	19970205		
PRIORITY APPLN. INFO.:			JP 1986-300810	19861217

OTHER SOURCE(S): MARPAT 110:75160
GI

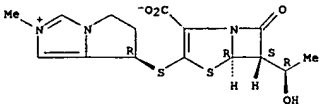


AB The title compds. (I; R1 = pyrrolidinoimidazole Q, Q1; R2 = ester residue, H, or CO2R2 = CO2-; R3 = H, (mono- or di-loweralkyl)carbamoyl, lower alkoxy carbamoyl, morpholinocarbonyl, (un)substituted imidazolyl, (un)substituted thiazolyl, acyl, halo, lower alkyl, lower alkoxy, cycloalkyl, Ph, etc.) were prepared as antibacterials. A solution of 250 mg p-nitrobenzyl (5R,6S,8R)-2-ethylsulfinyl-6-(1-hydroxyethyl)-2-penem-3-carboxylate in DMF was cooled to -40° and a solution of 440 mg 6,7-dihydro-7-mercapto-5H-pyrrolo[1,2-c]imidazole-CF3SO3H in DMF followed by (iso-Pr)2NEt was added. The resulting mixture was stirred at the same temperature for 30 min to give 290 mg (5R,6S,8R)-I [R1 = 6,7-dihydro-5H-pyrrolo[1,2-c]imidazol-7-yl, R2 = p-O2NC6H4CH2] which was hydrogenolized over Pd/C in THF-phosphate buffer to give an isomeric mixture of (5R,6S,8R)-I (R1 = the same as above, R2 = H). One of the above isomers showed a min. inhibitory concentration of ≤0.05 μg/mL against Staphylococcus aureus.
IT **108308-24-3P 108308-25-4P 108308-41-4P**
108308-42-5P 108308-46-9P 108308-47-0P
118776-44-6P 118776-73-1P 118776-75-3P
118776-76-4P 118776-77-5P 118776-78-6P
118776-79-7P 118776-80-0P 118776-81-1P
118776-82-2P 118776-83-3P 118776-84-4P
118776-85-5P 118776-86-6P 118776-87-7P
118776-89-9P 118776-90-2P 118776-91-3P

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
118776-92-4P 118776-93-5P 118776-94-6P
118776-95-7P 118776-96-8P 118776-97-9P
118776-98-0P 118776-99-1P 118777-00-7P
118777-01-8P 118777-02-9P 118859-84-0P
118866-55-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of, as antibacterial)

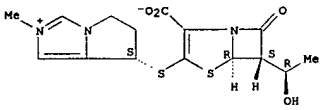
RN 108308-24-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-25-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

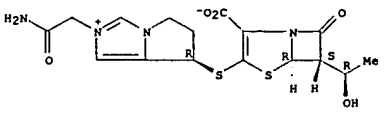
Absolute stereochemistry.



RN 108308-41-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

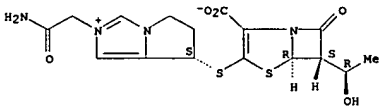
Absolute stereochemistry.

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



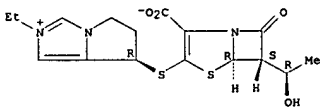
RN 108308-42-5 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-46-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-ethyl-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-47-0 HCAPLUS
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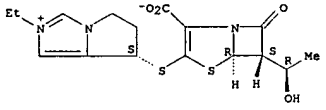
Absolute stereochemistry.

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 118776-44-6 HCAPLUS
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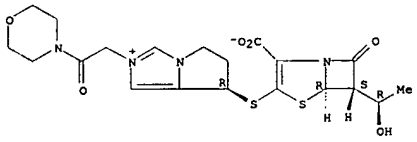
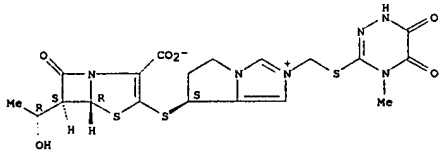
Absolute stereochemistry.



RN 118776-73-1 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[[(1,4,5,6-tetrahydro-4-methyl-5,6-dioxo-1,2,4-triazin-3-yl)thio]methyl]-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

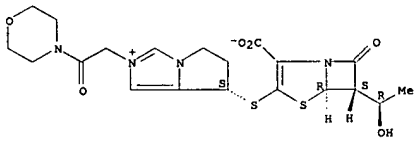
Absolute stereochemistry.



RN 118776-75-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[2-(4-morpholinyl)-2-oxoethyl]-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

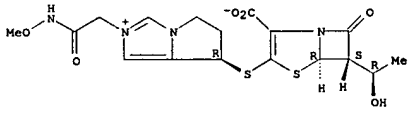
Absolute stereochemistry.

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



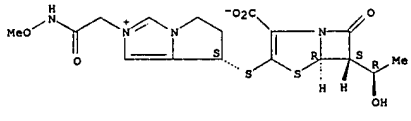
RN 118776-76-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[2-(methoxyamino)-2-oxoethyl]-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



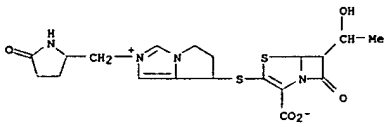
RN 118776-77-5 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[2-(methoxyamino)-2-oxoethyl]-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



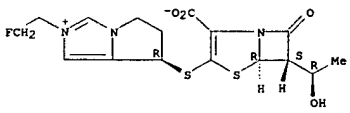
RN 118776-78-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[(5-oxo-2-pyrrolidinyl)methyl]-, inner salt, [5R-[3[R*(S*)],5α,6α(R*)]]- (9CI) (CA INDEX NAME)

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



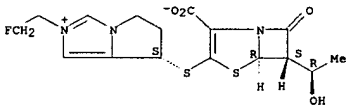
RN 118776-79-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-(2-fluoroethyl)-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 118776-80-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-(2-fluoroethyl)-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

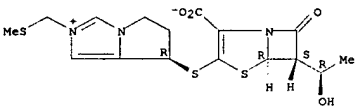
Absolute stereochemistry.



RN 118776-81-1 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-methoxyethyl)-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 118776-85-5 HCAPLUS
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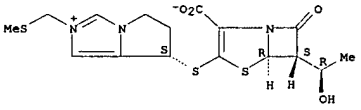
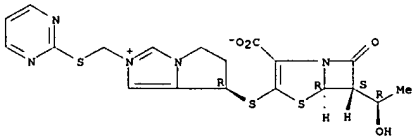
Absolute stereochemistry.



RN 118776-86-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[(2-pyrimidinylthio)methyl]-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

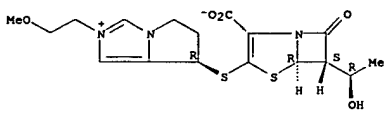
Absolute stereochemistry.



RN 118776-87-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[(2-pyrimidinylthio)methyl]-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 118776-82-2 HCAPLUS
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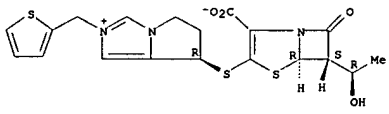
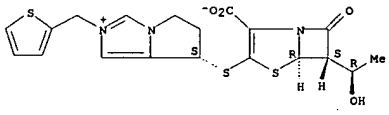
Absolute stereochemistry.



RN 118776-83-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-thienylmethyl)-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

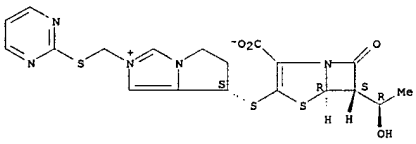
Absolute stereochemistry.



RN 118776-84-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[(methylthio)methyl]-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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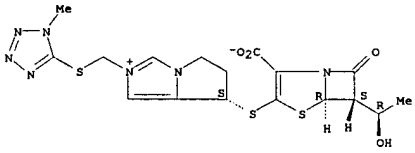
Absolute stereochemistry.



RN 118776-90-2 HCAPLUS
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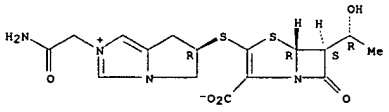
Absolute stereochemistry.



RN 118776-91-3 HCAPLUS
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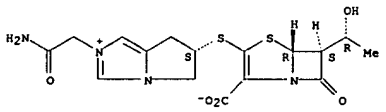
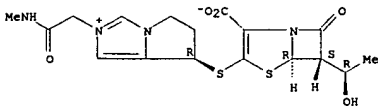
Absolute stereochemistry.

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



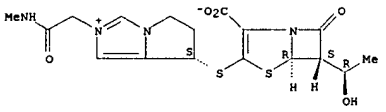
RN 118776-92-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[2-(methylamino)-2-oxoethyl]-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 118776-93-5 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[2-(methylamino)-2-oxoethyl]-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

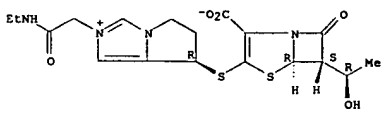
Absolute stereochemistry.



RN 118776-94-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-[2-(ethylamino)-2-oxoethyl]-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

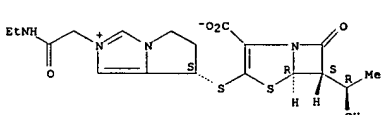
Absolute stereochemistry.

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



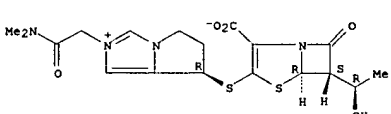
RN 118776-95-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-[2-(ethylamino)-2-oxoethyl]-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 118776-96-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-[2-(dimethylamino)-2-oxoethyl]-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

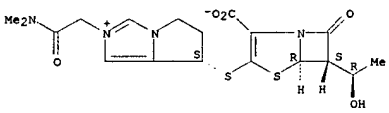
Absolute stereochemistry.



RN 118776-97-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-[2-(dimethylamino)-2-oxoethyl]-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

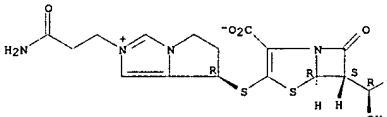
Absolute stereochemistry.

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



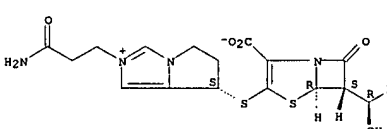
RN 118776-98-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(3-amino-3-oxopropyl)-7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 118776-99-1 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(3-amino-3-oxopropyl)-7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

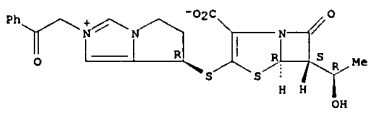
Absolute stereochemistry.



RN 118777-00-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-oxo-2-phenylethyl)-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

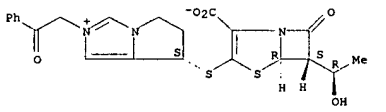
Absolute stereochemistry.

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



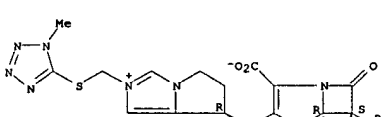
RN 118777-01-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-oxo-2-phenylethyl)-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 118777-02-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

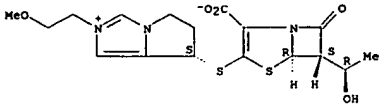
Absolute stereochemistry.



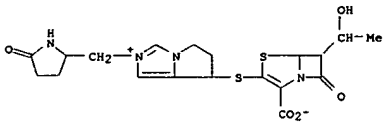
RN 118859-84-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-methoxyethyl)-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

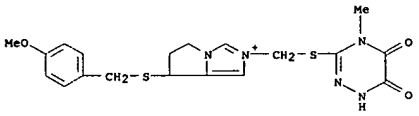
L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 118866-55-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[(5-oxo-2-pyrrolidinyl)methyl]-, inner salt, [5R-[3[S*(S*)],5α,6α(R*)]]- (9CI) (CA INDEX NAME)



IT 118776-36-6P 118776-38-8P 118776-54-8P
118776-56-0P 118776-57-1P 118776-59-3P
118776-60-6P 118776-62-8P 118776-63-9P
118776-65-1P 118776-66-2P 118776-68-4P
118776-70-8P 118776-72-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for penem antibacterial)
RN 118776-36-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-[[(4-methoxyphenyl)methyl]thio]-2-[[(1,4,5,6-tetrahydro-4-methyl-5,6-dioxo-1,2,4-triazin-3-yl)thio]methyl]-, iodide (9CI) (CA INDEX NAME)



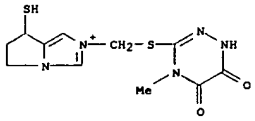
● I⁻

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 118776-38-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-mercapto-2-[[(1,4,5,6-tetrahydro-4-methyl-5,6-dioxo-1,2,4-triazin-3-yl)thio]methyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

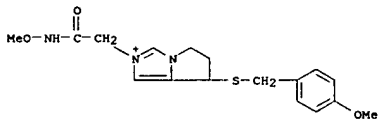
CRN 118776-37-7
CMF C11 H14 N5 O2 S2



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 118776-54-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-2-[2-(methoxyamino)-2-oxoethyl]-7-[[(4-methoxyphenyl)methyl]thio]-, bromide (9CI) (CA INDEX NAME)



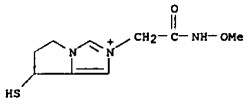
● Br⁻

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 118776-56-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-mercapto-2-[2-(methoxyamino)-2-oxoethyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

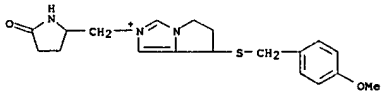
CRN 118776-55-9
CMF C9 H14 N3 O2 S



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 118776-57-1 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-[[(4-methoxyphenyl)methyl]thio]-2-[(5-oxo-2-pyrrolidinyl)methyl]-, iodide (9CI) (CA INDEX NAME)



● I⁻

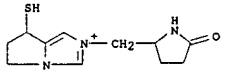
RN 118776-59-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-mercapto-2-[(5-oxo-2-

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

pyrrolidinyl)methyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

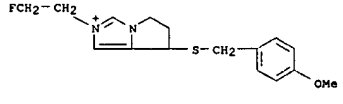
CRN 118776-58-2
CMF C11 H16 N3 O S



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 118776-60-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-fluoroethyl)-6,7-dihydro-7-[[(4-methoxyphenyl)methyl]thio]-, bromide (9CI) (CA INDEX NAME)



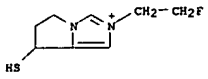
● Br⁻

RN 118776-62-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-fluoroethyl)-6,7-dihydro-7-mercapto-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 118776-61-7
CMF C8 H12 F N2 S

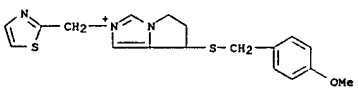
L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 118776-63-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-[[(4-methoxyphenyl)methyl]thio]-2-(2-thiazolylmethyl)-, chloride (9CI) (CA INDEX NAME)



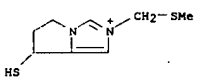
● Cl⁻

RN 118776-65-1 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-mercapto-2-(2-thiazolylmethyl)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 118776-64-0
CMF C10 H12 N3 S2

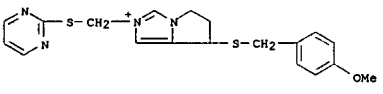
L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 118776-70-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-[[(4-methoxyphenyl)methyl]thio]-2-[(2-pyrimidinylthio)methyl]-, iodide (9CI) (CA INDEX NAME)

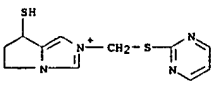


● I⁻

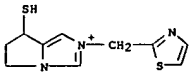
RN 118776-72-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-mercapto-2-[(2-pyrimidinylthio)methyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 118776-71-9
CMF C11 H13 N4 S2



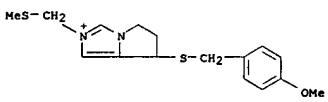
L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 118776-66-2 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-[[(4-methoxyphenyl)methyl]thio]-2-[(methylthio)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

RN 118776-68-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-mercapto-2-[(methylthio)methyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 118776-67-3
CMF C8 H13 N2 S2

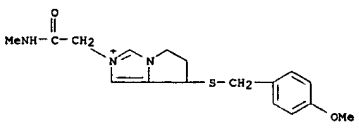
L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 37181-39-8
CMF C F3 O3 S

IT 118776-45-7P 118776-47-9P 118776-48-0P
118776-50-4P 118776-52-6P 118776-88-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for penem antibacterials)

RN 118776-45-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-[[(4-methoxyphenyl)methyl]thio]-2-[2-(methylamino)-2-oxoethyl]-, bromide (9CI) (CA INDEX NAME)



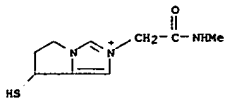
● Br⁻

RN 118776-47-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-mercapto-2-[2-(methylamino)-2-oxoethyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 118776-46-8
CMF C9 H14 N3 O S

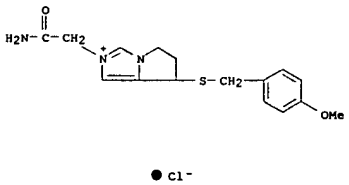
L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 118776-48-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-6,7-dihydro-7-[[(4-methoxyphenyl)methyl]thio]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

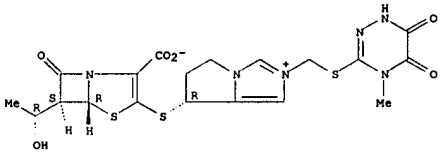
RN 118776-50-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-6,7-dihydro-7-mercapto-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

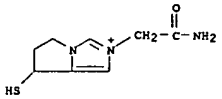
CRN 118776-49-1
CMF C8 H12 N3 O S

L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-[[(1,4,5,6-tetrahydro-4-methyl-5,6-dioxo-1,2,4-triazin-3-yl)thio]methyl]-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L69 ANSWER 37 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



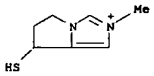
CM 2

CRN 37181-39-8
CMF C F3 O3 S

RN 118776-52-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-mercapto-2-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 118776-51-5
CMF C7 H11 N2 S

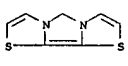


CM 2

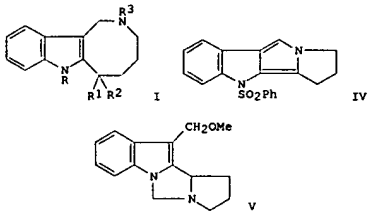
CRN 37181-39-8
CMF C F3 O3 S

RN 118776-88-8 HCAPLUS

L69 ANSWER 38 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:59768 HCAPLUS
DOCUMENT NUMBER: 108:59768
TITLE: Late Quaternary Mediterranean sapropels. II. Organic geochemistry and palynology of S1 sapropels and associated sediments
AUTHOR(S): Ten Haven, H. L.; Baas, M.; De Leeuw, J. W.; Schenck, P. A.; Brinkhuis, H.
CORPORATE SOURCE: Dep. Chem. Chem. Eng., Delft Univ. Technol., Delft, 2628 RZ, Neth.
SOURCE: Chemical Geology (1987), 64(1-2), 149-67
CODEN: CHGEAD; ISSN: 0009-2541
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The organic matter of S1 sapropels is of a mixed marine, terrigenous, and bacterial origin. A trend of relatively increasing amts. of continent-derived organic matter towards more seaward and deeper realms can be observed from both palynol. and organic geochem. data. This trend is supported to some extent by δ13C-values of the organic matter. The sapropelic intervals deposited on the Nile Cone are characterized by expanded thicknesses and a diluted organic C content because of a higher sedimentation rate. The environmental conditions (in terms of preservation) during sapropel formation over the eastern Mediterranean were probably not uniform. At site 29, the conditions were favorable for the deposition of sapropel with a higher organic C content than at the other locations. This might have been caused by better preservation conditions. Increasing discharge from the Nile River was the driving force for formation of the S1 sapropels. Based on this assumption a model for sapropel formation is proposed.
IT 236-71-5
RL: GOC (Geological or astronomical occurrence); OCCU (Occurrence) (in sapropels, of late Quaternary, of eastern Mediterranean)
RN 236-71-5 HCAPLUS
CN 5H-Imidazo[5,1-b:4,3-b']bisthiazole (8CI, 9CI) (CA INDEX NAME)

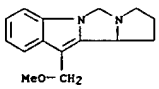


L69 ANSWER 39 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:55922 HCAPLUS
DOCUMENT NUMBER: 108:55922
TITLE: Synthesis of some hexahydroazocino[4,3-b]indoles, a tetra- and two hexahydropyrrolo[1',2':1,2]pyrrolo[3,4-b]indoles, and a tetrahydropyrrolo[2',1':5,1]imidazo[3,4-a]indole. Crystal structure determination of 1,2,3,4-tetrahydro-2-(phenoxycarbonyl)-7-(phenylsulfonyl)azocino[4,3-b]indol-6(5H)-one
AUTHOR(S): Street, Jonathan D.; Harris, Martin; Bishop, David I.; Heatley, Frank; Beddoes, Roy L.; Mills, Owen S.; Joule, John A.
CORPORATE SOURCE: Chem. Dep., Univ. Manchester, Manchester, M13 9PL, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (7), 1599-606
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:55922
GI



AB Azocinoindoles I (R = H, SO2Ph; R1 = H, R2 = OH; R1R2 = O; R3 = CH2Ph) were prepared from 1-phenylsulfonylindole by introducing the appropriate side chain at C-2 via lithiation, and then intramol. Mannich cyclization. I (R = SO2Ph, R1R2 = O, R = CO2Ph, II) was prepared from I (R = SO2Ph, R1R2 = O, R3 = CH2Ph, III). The mol. structure of II was determined by x-ray crystal structure anal. The benzyl group of II was also replaced by other urethane groups. Cleavage of the urethanes gave pyrrolopyrroloindoles, e.g., IV. Reaction of 2-indol-2-ylpyrrolidine with CH2O in methanolic methoxide gave pyrroloimidazoindole V.
IT 112565-43-2P

L69 ANSWER 39 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 112565-43-2 HCAPLUS
CN 5H-Pyrrolo[1',2':3,4]imidazo[1,5-a]indole, 1,2,3,11b-tetrahydro-11-(methoxymethyl)- (9CI) (CA INDEX NAME)

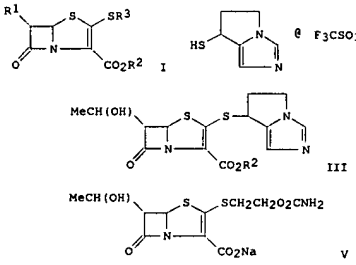


L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:213640 HCAPLUS
DOCUMENT NUMBER: 106:213640
TITLE: Heterocyclylthio derivatives of penemcarboxylic acid and their use as antibacterials
INVENTOR(S): Sato, Makoto; Takemura, Makoto; Higashi, Kunio; Soga, Tsunehiko; Matsumoto, Hiroo; Nishi, Toshiyuki
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 180 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 210883	A2	19870204	EP 1986-401308	19860617
EP 210883	A3	19870701		
EP 210883	B1	19950201		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
CA 1339860	A1	19980512	CA 1986-511536	19860613
ZA 8604472	A	19870225	ZA 1986-4472	19860616
DK 8602835	A	19861218	DK 1986-2835	19860617
DK 171644	B1	19970303		
FI 8602566	A	19861218	FI 1986-2566	19860617
FI 87218	B	19920831		
FI 87218	C	19921210		
NO 8602411	A	19861218	NO 1986-2411	19860617
NO 167982	B	19910923		
NO 167982	C	19920102		
AU 8658909	A1	19861224	AU 1986-58909	19860617
AU 593558	B2	19900215		
JP 62149683	A2	19870703	JP 1986-141171	19860617
JP 08026040	B4	19960313		
ES 556137	A1	19880101	ES 1986-556137	19860617
US 4962202	A	19901009	US 1988-117617	19880111
AU 8944784	A1	19900308	AU 1989-44784	19891117
AU 626606	B2	19920806		
US 5079357	A	19920107	US 1989-449391	19891207
JP 06184146	A2	19940705	JP 1993-145807	19930617
PRIORITY APPLN. INFO.:			JP 1985-131394	A 19850617
			JP 1985-213420	A 19850926
			US 1986-875228	B2 19860617
			US 1987-38640	B3 19870415

OTHER SOURCE(S): MARPAT 106:213640
GI

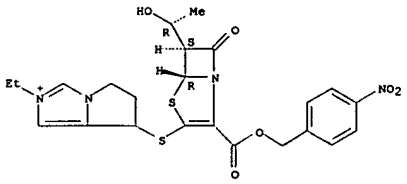
L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB Penem derivs. I [R1 = H, alkyl, hydroxyalkyl; CO2R2 = CO2H, CO2-; R2 = ester group, protective group; R3 = (un)substituted bicycloheterocyclyl] and their salts, useful as antibacterial agents with extremely wide antibacterial spectrum, were prepared by reacting 2-substituted sulfinyl derivs. of penem with HSR3 and then optionally removing protective group(s) and further alkylating the reaction product or vice versa. Et urocanate-HCl was alkalinated and reacted with 4-MeOC6H4CH2SH and the product Et 3-(imidazol-4-yl)-3-(p-methoxybenzylthio)propionate was converted in 4 steps to pyrroloimidazole salt II. This reacted with p-nitrobenzyl (5R,6S,8R)-2-ethylsulfinyl-6-(1-hydroxyethyl)-2-penem-3-carboxylate to give the sulfide (5R,6S,8R)-III (R2 = 4-O2NC6H4CH2), hydrogenolysis of which over 10% Pd/C gave (5R,6S,8R)-III (R = H) (IV) as isomers A and B. The min. inhibitory concentration of isomer A of IV against E. coli N1HJ was 0.1 μg/mL, whereas that of carbamate V was 0.39 μg/mL.
IT 108308-48-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 108308-48-1 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-ethyl-6,7-dihydro-7-[[6-(1-hydroxyethyl)-2-[[(4-nitrophenyl)methoxy]carbonyl]-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-, iodide, [5R-[5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

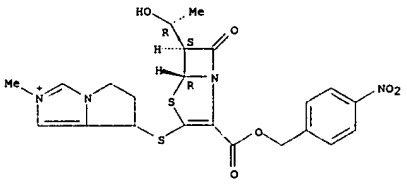
L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● I⁻

IT 108308-26-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 108308-26-5 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-[[6-(1-hydroxyethyl)-2-[[(4-nitrophenyl)methoxy]carbonyl]-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-methyl-, iodide, [5R-[5α,6α(R*)]]- (9CI) (CA INDEX NAME)

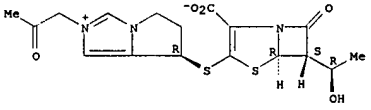
Absolute stereochemistry.



● I⁻

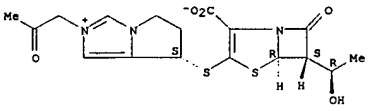
IT 108308-24-3P 108308-25-4P 108308-27-6P
108308-28-7P 108308-29-8P 108308-30-1P
108308-31-2P 108308-32-3P 108308-33-4P

L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



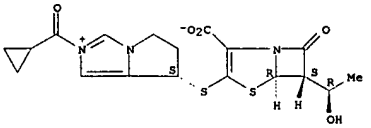
RN 108308-28-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 5-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-oxopropyl)-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-29-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-(cyclopropylcarbonyl)-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



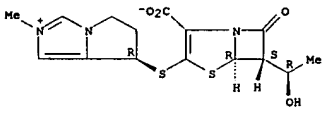
RN 108308-30-1 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(cyclopropylcarbonyl)-6,7-dihydro-7-[[6-(1-hydroxyethyl)-2-[[(4-nitrophenyl)methoxy]carbonyl]-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-, iodide, [5R-[5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

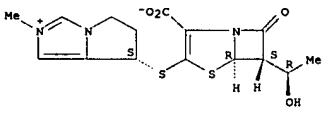
108308-34-5P 108308-35-6P 108308-36-7P
108308-37-8P 108308-38-9P 108308-39-0P
108308-40-3P 108308-41-4P 108308-42-5P
108308-43-6P 108308-44-7P 108308-45-8P
108308-46-9P 108308-47-0P 108308-49-2P
108308-50-5P 108308-51-6P 108308-52-7P
108309-32-6P 108309-33-7P 108325-51-5P
108325-52-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of, as antibacterial)
RN 108308-24-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-25-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

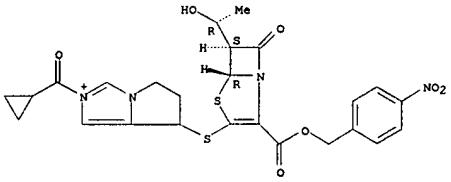
Absolute stereochemistry.



RN 108308-27-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 5-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-oxopropyl)-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

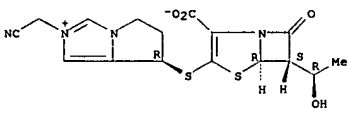
L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● I⁻

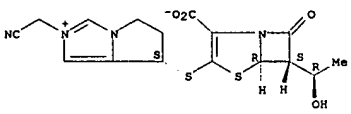
RN 108308-31-2 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-(cyanomethyl)-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-32-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-(cyanomethyl)-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

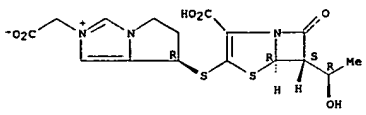
Absolute stereochemistry.



RN 108308-33-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-

L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
, inner salt, monosodium salt, [5R-[3(R*),5α,6α(R*)]]- (9CI)
(CA INDEX NAME)

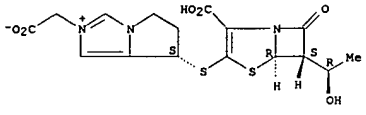
Absolute stereochemistry.



● Na

RN 108308-34-5 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-(carboxymethyl)-6,7-dihydro-, inner salt, monosodium salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

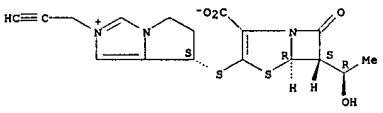


● Na

RN 108308-35-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-propenyl)-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

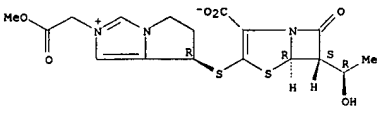
Absolute stereochemistry.

L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



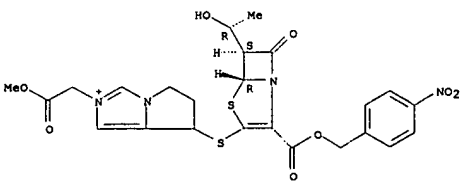
RN 108308-39-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-methoxy-2-oxoethyl)-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-40-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6,7-dihydro-7-[[6-(1-hydroxyethyl)-2-[[(4-nitrophenyl)methoxy]carbonyl]-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-(2-methoxy-2-oxoethyl)-, bromide, [5R-[5α,6α(R*)]]- (9CI) (CA INDEX NAME)

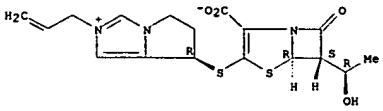
Absolute stereochemistry.



● Br⁻

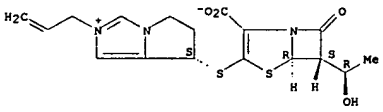
RN 108308-41-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-7-[[2-carboxy-6-(1-

L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



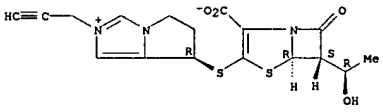
RN 108308-36-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-propenyl)-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-37-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-propynyl)-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

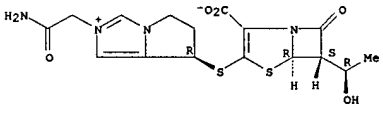


RN 108308-38-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-propynyl)-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

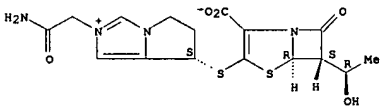
L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-42-5 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-(2-amino-2-oxoethyl)-7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

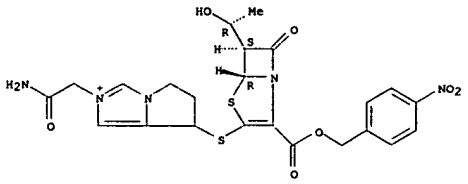
Absolute stereochemistry.



RN 108308-43-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium,
2-(2-amino-2-oxoethyl)-6,7-dihydro-7-[[6-(1-hydroxyethyl)-2-[[(4-nitrophenyl)methoxy]carbonyl]-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-, iodide, [5R-[5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

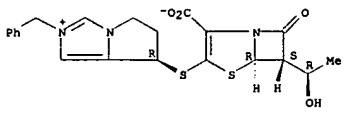
L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● I⁻

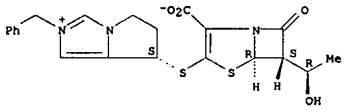
RN 108308-44-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(phenylmethyl)-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-45-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(phenylmethyl)-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

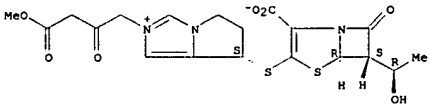
Absolute stereochemistry.



L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

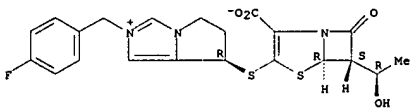
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(4-methoxy-2,4-dioxobutyl)-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



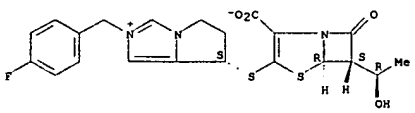
RN 108308-51-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-[(4-fluorophenyl)methyl]-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-52-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-[(4-fluorophenyl)methyl]-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

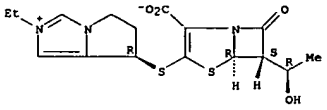


RN 108309-32-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

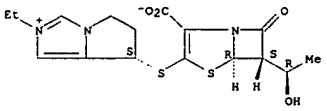
RN 108308-46-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-ethyl-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



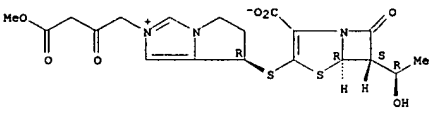
RN 108308-47-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-ethyl-6,7-dihydro-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108308-49-2 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(4-methoxy-2,4-dioxobutyl)-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

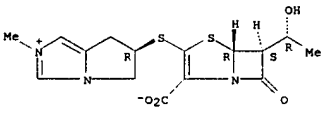
Absolute stereochemistry.



RN 108308-50-5 HCAPLUS

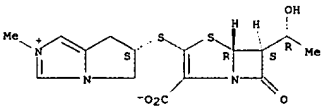
L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.



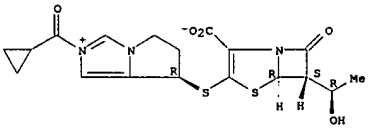
RN 108309-33-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 108325-51-5 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-2-(cyclopropylcarbonyl)-6,7-dihydro-, inner salt, [5R-[3(R*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

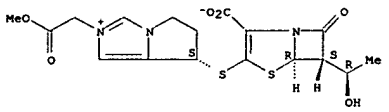
Absolute stereochemistry.



RN 108325-52-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-(2-methoxy-2-oxoethyl)-, inner salt, [5R-[3(S*),5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L69 ANSWER 40 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L69 ANSWER 41 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

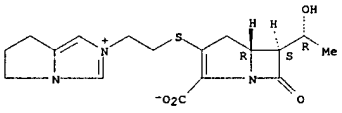
ACCESSION NUMBER: 1987:67000 HCAPLUS
DOCUMENT NUMBER: 106:67000
TITLE: Carbapenems having a 2-quaternary hetero-arylalkylthio substituent
INVENTOR(S): Christensen, Burton G.; Johnston, David B. R.; Schmitt, Susan M.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Eur. Pat. Appl., 194 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 169410	A1	19860129	EP 1985-108133		19850701
EP 169410	B1	19930224			
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE					
CA 1285940	A1	19910709	CA 1985-486090		19850628
DK 8502974	A	19860314	DK 1985-2974		19850701
ES 544753	A1	19860916	ES 1985-544753		19850701
AT 85978	E	19930315	AT 1985-108133		19850701
JP 61083184	A2	19860426	JP 1985-145660		19850702
PRIORITY APPLN. INFO.:			US 1984-626580	A	19840702
			EP 1985-108133	A	19850701

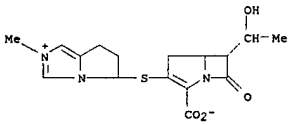
GI For diagram(s), see printed CA Issue.
AB The title compds. I [L = (un)substituted C1-6 alkyl, C2-6 alkenyl, C3-6 cycloalkyl, etc.; X completes an (un)substituted mono- or bicyclic heterocyclyl; Y = CO2H, CO2R; R = removable CO2H protecting group, CO2M; M = alkali metal], their esters and salts, useful as antibiotics (no data) were prepared Thus, p-nitrobenzyl (5R,6S)-2-[(diphenylphosphono)oxy]-6-[1(R)-hydroxyethyl]carbapen-2-em-3-carboxylate in MeCN was treated with 1-(2-mercaptoethyl)pyridinium nitrate in DMSO and with EtN(CHMe2)2 to give (5R,6S)-6-[1(R)-hydroxyethyl]-2-[(2-pyridinioethyl)thio]carbapen-2-em-3-carboxylate.
IT **104262-91-1P 104285-15-6P 104285-16-7P 104285-17-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibiotic)
RN 104262-91-1 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-[2-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]ethyl]-6,7-dihydro-, inner salt, [5R-[5α,6α(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

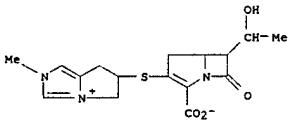
L69 ANSWER 41 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 104285-15-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 5-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt (9CI) (CA INDEX NAME)

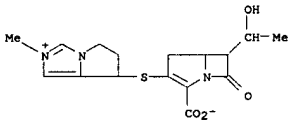


RN 104285-16-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt (9CI) (CA INDEX NAME)



RN 104285-17-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt (9CI) (CA INDEX NAME)

L69 ANSWER 41 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

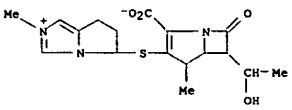


L69 ANSWER 42 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:66999 HCAPLUS
DOCUMENT NUMBER: 106:66999
TITLE: 1-Methylcarbapenems having a 2-quaternary heteroarylalkylthio substituent
INVENTOR(S): Christensen, Burton G.; Johnston, David B. R.; Schmitt, Susan M.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Eur. Pat. Appl., 203 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

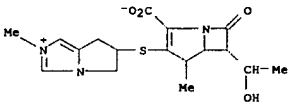
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 168707	A1	19860122	EP 1985-108134	19850701
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
CA 1273013	A1	19900821	CA 1985-486070	19850628
DK 8502976	A	19860103	DK 1985-2976	19850701
ES 544754	A1	19860916	ES 1985-544754	19850701
JP 61063679	A2	19860401	JP 1985-145661	19850702
PRIORITY APPLN. INFO.:			US 1984-626822 A	19840702

GI For diagram(s), see printed CA Issue.
AB The title compds. I (L = (un)substituted C1-6 alkyl, C2-6 alkenyl, C3-6 cycloalkyl, etc.; X completes an (un)substituted mono- or bicyclic heterocycle; Y = CO2H, CO2R; R = removable protecting group, CO2M; M = alkali metal), their esters and salts, useful as antibiotics (no data), were prepared Thus, p-nitrobenzyl (5S,6S)-2-[(diphenylphosphono)oxy]-6-[1(R)-hydroxyethyl]-1(R)-methylcarbapen-2-em-3-carboxylate and 3-hydroxy-1-(mercaptoethyl)pyridinium nitrate in MeCONMe2 was treated with EtNPr2-iso2, then diluted with BuOH, EtOAc, and H2O, the pH adjusted with N-methylmorpholine-HCl, treated with Pd(OH)2/C and hydrogenated to give Na (5S,6S)-6-[1(R)-hydroxyethyl]-1(R)-methyl-2-[2-(3-oxidopyridinium)ethylthio]carbapen-2-em-3-carboxylate.
IT **103911-25-7P 103911-26-8P 103911-27-9P 103965-56-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibiotic)
RN 103911-25-7 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 5-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt (9CI) (CA INDEX NAME)

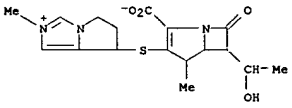
L69 ANSWER 42 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 103911-26-8 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 6-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt (9CI) (CA INDEX NAME)

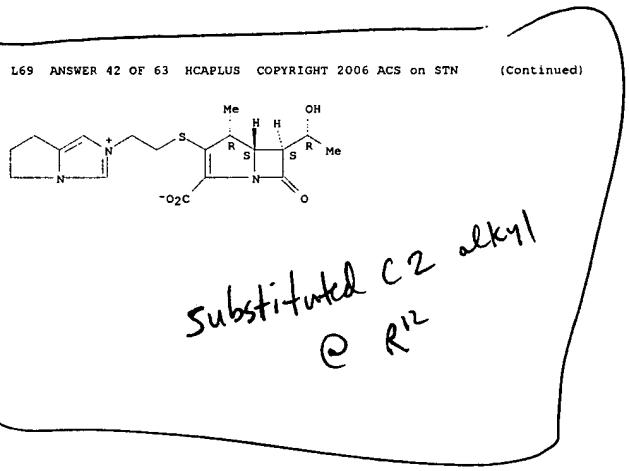


RN 103911-27-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 7-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]-6,7-dihydro-2-methyl-, inner salt (9CI) (CA INDEX NAME)

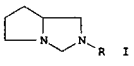


RN 103965-56-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazolium, 2-[2-[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]thio]ethyl]-6,7-dihydro-, inner salt, [4R-[4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

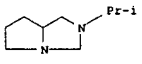
Absolute stereochemistry.



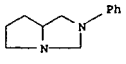
L69 ANSWER 43 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:5820 HCAPLUS
DOCUMENT NUMBER: 104:5820
TITLE: Lithium aluminum hydride reduction with a ring closure. A facile synthesis of 1,3-dialkylimidazolidines and 1,3-disubstituted 4-imidazolines from α-amino acid derivatives
AUTHOR(S): Kiyooka, Syunichi; Goto, Fumitaka; Fujiyama, Ryoji; Suzuki, Kojiro
CORPORATE SOURCE: Fac. Sci., Kochi Univ., Kochi, 780, Japan
SOURCE: Kochi Daigaku Rigakubu Kiyo, Kagaku (1985), 6, 15-20
CODEN: KDRKDD; ISSN: 0389-0279
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



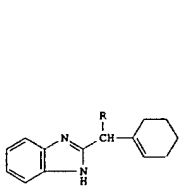
AB N-Isopropyl-N-(benzyloxycarbonyl)prolinamide was treated with LiAlH4 in THF to give 3-isopropyl-1,3-diazabicyclo[3.3.0]octane (I; R = Me2CH). Similarly, N-isopropyl-N-(benzyloxycarbonyl)sarcosinamide and N-phenyl-N-(benzyloxycarbonyl)prolinamide gave 1-isopropyl-3-methylimidazolidine and 3-phenyl-1,3-diazabicyclo[3.3.0]octane (I; R = Ph), resp.
IT **99405-62-6P 99405-64-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 99405-62-6 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole, hexahydro-2-(1-methylethyl)- (9CI) (CA INDEX NAME)



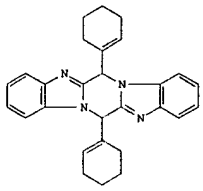
RN 99405-64-8 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole, hexahydro-2-phenyl- (9CI) (CA INDEX NAME)



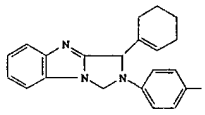
L69 ANSWER 44 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:78770 HCAPLUS
DOCUMENT NUMBER: 102:78770
TITLE: Benzimidazole derivatives. XII. Reactions of 2-(α-chloro-3',4',5',6'-tetrahydrobenzyl)benzimidazole with phenols and aromatic amines
AUTHOR(S): Saczewski, Franciszek; Foks, Henryk; Sawlewicz, Jozef
CORPORATE SOURCE: Inst. Technol. Anal. Pharm. Prod., Sch. Med., Gdansk, 80-416, Pol.
SOURCE: Acta Poloniae Pharmaceutica (1984), 41(1), 31-6
CODEN: APPHAX; ISSN: 0001-6837
DOCUMENT TYPE: Journal
LANGUAGE: Polish
OTHER SOURCE(S): CASREACT 102:78770
GI



I

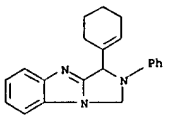


III

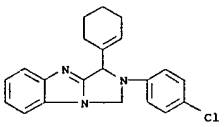


IV

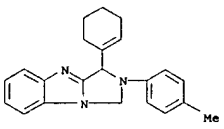
AB The title benzimidazole derivative (I, R = Cl) with R1ONa (R1 = Ph, C6H4Cl-4, C6H4NH2-4) in MeOH gave I (R = OR1). A similar reaction with 4-R2C6H4NH2 (R2 = H, Cl, Me) in the presence of Et3N yielded I (R = NHC6H4R2) (II). I.HCl (R = Cl) with Et3N in DMF yielded the dimer III. A 1,3-dipole was the intermediate in the investigated reactions. Cyclocondensation of II with CH2O in EtOH gave the corresponding imidazobenzimidazoles IV.
IT **94640-89-8P 94640-90-1P 94640-91-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 94640-89-8 HCAPLUS
CN 1H-Imidazo[1,5-a]benzimidazole, 3-(1-cyclohexen-1-yl)-2,3-dihydro-2-phenyl- (9CI) (CA INDEX NAME)



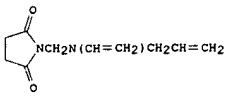
RN 94640-90-1 HCAPLUS
CN 1H-Imidazo[1,5-a]benzimidazole, 2-(4-chlorophenyl)-3-(1-cyclohexen-1-yl)-2,3-dihydro- (9CI) (CA INDEX NAME)



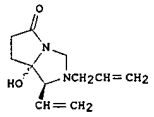
RN 94640-91-2 HCAPLUS
CN 1H-Imidazo[1,5-a]benzimidazole, 3-(1-cyclohexen-1-yl)-2,3-dihydro-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



L69 ANSWER 45 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:103247 HCAPLUS
DOCUMENT NUMBER: 100:103247
TITLE: Synthesis of diazaheterocycles with a bridgehead nitrogen by photocyclization of N-substituted alicyclic imides
AUTHOR(S): Coyle, John D.; Bryant, Laurence R. B.
CORPORATE SOURCE: Chem. Dep., Open Univ., Milton Keynes, MK7 6AA, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1983), (12), 2857-65
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:103247
GI

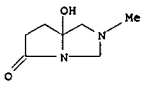


I



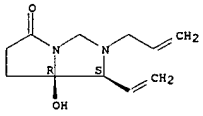
II

AB N-(Dialkylaminomethyl)succinimides and -glutarimides cyclized to 1,3-diazabicyclo[3.3.0]octanes and -[4.3.0]nonanes, resp., on irradiation in MeCN. E.g., irradiation of succinimide I in MeCN gave 26 and 20% yields of the 2 diastereoisomers of diazabicyclooctanes II. N-(Dialkylaminoethyl) aliphatic imides gave azepine- or azocinediones on irradiation, whereas N-(dialkylaminopropyl) derivs. cyclized to give products with a novel perhydro-1,4-diazepine ring. Cyclization of N-(dialkylaminoethyl)maleimide and the analogous 3,4,5,6-tetrahydrophthalimide gave compds. containing a new piperazine ring.
IT **89003-45-2P 89003-46-3P 89003-47-4P 89003-48-5P 89003-49-6P 89003-50-9P 89003-51-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 89003-45-2 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazol-5-one, hexahydro-7a-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



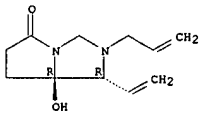
RN 89003-46-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazol-5-one, 1-ethenylhexahydro-7a-hydroxy-2-(2-propenyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



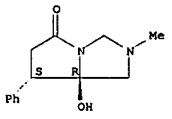
RN 89003-47-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazol-5-one, 1-ethenylhexahydro-7a-hydroxy-2-(2-propenyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 89003-48-5 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazol-5-one, hexahydro-7a-hydroxy-2-methyl-7-phenyl-, trans- (9CI) (CA INDEX NAME)

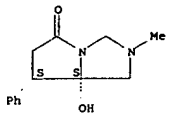
Relative stereochemistry.



RN 89003-49-6 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazol-5-one, hexahydro-7a-hydroxy-2-methyl-7-phenyl-,

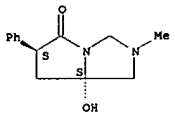
L69 ANSWER 45 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



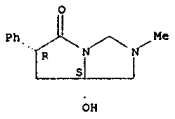
RN 89003-50-9 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazol-5-one, hexahydro-7a-hydroxy-2-methyl-6-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 89003-51-0 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazol-5-one, hexahydro-7a-hydroxy-2-methyl-6-phenyl-, cis- (9CI) (CA INDEX NAME)

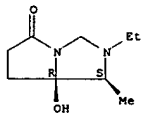
Relative stereochemistry.



IT **83095-08-3P 83095-09-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by photocyclization of (dialkylaminomethyl)succinimide)
RN 83095-08-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazol-5-one, 2-ethylhexahydro-7a-hydroxy-1-methyl-, cis- (9CI) (CA INDEX NAME)

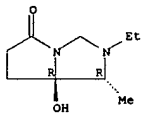
Relative stereochemistry.

L69 ANSWER 45 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

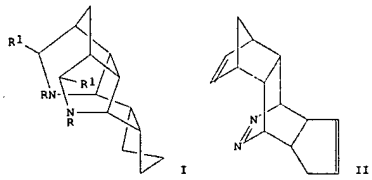


RN 83095-09-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazol-5-one, 2-ethylhexahydro-7a-hydroxy-1-methyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L69 ANSWER 46 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:34517 HCAPLUS
DOCUMENT NUMBER: 100:34517
TITLE: Preparation of some polycyclic diamine derivatives
AUTHOR(S): Nelsen, Stephen F.; Willi, Mark R.
CORPORATE SOURCE: S. M. McElvain Lab. Org. Chem., Univ. Wisconsin, Madison, WI, 53706, USA
SOURCE: Journal of Organic Chemistry (1984), 49(1), 1-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:34517
GI



I II

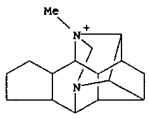
AB Diazahexacyclohexadecanes I (R = H, Cl, Me, NO, NH2, NMe2, NEt2; R12 = bond) and the related pentacyclic compds. lacking the 2,12 C-C bond were prepared from cyclopentadiene and 2,5-dimethoxy-2,5-dihydrofuran via photolysis of II. Mol. mechanics calcns. on I (R = Me, R12 = bond, R1 = H) are discussed.

IT **87801-37-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 87801-37-4 HCAPLUS
CN 2H-1,5,2,4-(Methanonitrilometheno)dicyclopent[cd,g]indolium, dodecahydro-1-methyl-, (1α,2α,2aβ,4α,4aβ,5.alpha.,5aβ,8aβ,8bβ,8cβ,9S*)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 87801-36-3
CMF C16 H23 N2

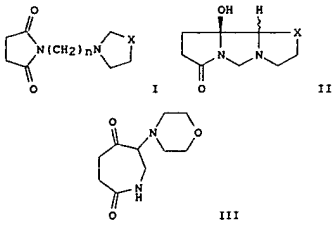
L69 ANSWER 46 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

L69 ANSWER 47 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:544818 HCAPLUS
DOCUMENT NUMBER: 97:144818
TITLE: Photocyclization of N-(dialkylaminoalkyl)succinimides
AUTHOR(S): Bryant, Laurence R. B.; Coyle, John D.
CORPORATE SOURCE: Dep. Chem., Open Univ., Milton Keynes, MK7 6AA, UK
SOURCE: Journal of Chemical Research, Synopses (1982), (6), 164-5
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:144818
GI

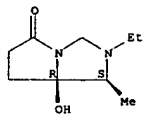


I II III

AB Photochem. cyclization of N-substituted succinimides I [n = 1, X = CH2O, CH:CH, (CH2)2, o-C6H4] in MeCN gave the diazabicyclooctanes II (X as before) in 46-77% yield. Irradiation of I [n = 2, X = CH2O] gave the azepine III in 46% yield.
IT **83095-08-3P 83095-09-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 83095-08-3 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazol-5-one, 2-ethylhexahydro-7a-hydroxy-1-methyl-, cis- (9CI) (CA INDEX NAME)

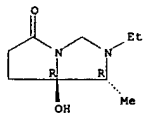
Relative stereochemistry.

L69 ANSWER 47 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

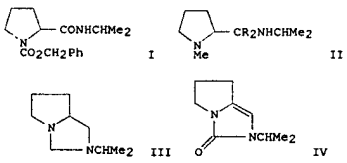


RN 83095-09-4 HCAPLUS
CN 5H-Pyrrolo[1,2-c]imidazol-5-one, 2-ethylhexahydro-7a-hydroxy-1-methyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



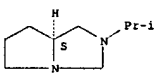
L69 ANSWER 48 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:7047 HCAPLUS
DOCUMENT NUMBER: 96:7047
TITLE: Solvent effect in the reaction of (S)-N-isopropyl-Nα-(benzyloxycarbonyl) prolinamide with lithium aluminum hydride
AUTHOR(S): Kiyooka, Syunichi; Goto, Fumitaka; Suzuki, Kojiro
CORPORATE SOURCE: Fac. Sci., Kochi Univ., Kochi, 780, Japan
SOURCE: Chemistry Letters (1981), (10), 1429-30
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II III IV

AB A specific solvent effect in the reduction of the title amide (I) with LiAlH4 was studied. The reactions in Et2O gave mainly II (R2 = O) and II (R = H), while III and IV were produced in THF.
IT **80090-66-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 80090-66-0 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole, hexahydro-2-(1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

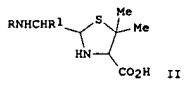
Absolute stereochemistry.



L69 ANSWER 49 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:170490 HCAPLUS
DOCUMENT NUMBER: 88:170490
TITLE: D-Penicillamine and its salts
INVENTOR(S): Sota, Kaoru; Ogawa, Toshihisa; Sawada, Jiro
PATENT ASSIGNEE(S): Taisho Pharmaceutical Co., Ltd., Japan
SOURCE: Ger. Offen., 20 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

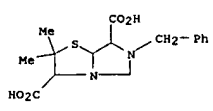
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2728870	A1	19780112	DE 1977-2728870	19770627
DE 2728870	C2	19850411		
JP 53007620	A2	19780124	JP 1976-82321	19760710
JP 56005389	B4	19810204		
JP 53084915	A2	19780726	JP 1976-158645	19761230
JP 55046390	B4	19801122		
GB 1523090	A	19780831	GB 1977-24800	19770614
US 4150240	A	19790417	US 1977-813989	19770708
CH 630070	A	19820528	CH 1977-8493	19770708
PRIORITY APPLN. INFO.:			JP 1976-82321 A	19760710
			JP 1976-158645 A	19761230

GI



II

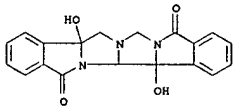
AB D-Penicillamine (I) was prepared by cleavage of II (R = H, PhCH2CO, PhOCH2CO; R1 = H, CO2H, CONH2, CONHPh, etc.) by aromatic amines. Thus, benzylpenicilloic acid α-phenethylamide was heated with (PhNHCH2)2 in aqueous AcOH, followed by acidification with HCl to give 82.8% I.HCl.
IT **66317-04-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring cleavage of, by aromatic amines)
RN 66317-04-2 HCAPLUS
CN Imidazo[5,1-b]thiazole-3,7-dicarboxylic acid, hexahydro-2,2-dimethyl-6-(phenylmethyl)- (9CI) (CA INDEX NAME)



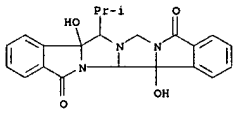
L69 ANSWER 49 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L69 ANSWER 50 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:443238 HCAPLUS
DOCUMENT NUMBER: 83:43238
TITLE: Photoreactions of bis(phthalimidomethyl)alkylamines
AUTHOR(S): Roth, H. J.; Schwarz, D.
CORPORATE SOURCE: Pharm. Inst., Univ. Bonn, Bonn, Fed. Rep. Ger.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1975), 308(3), 218-24
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB The condensed imidazoles I and II (R = H, CHMe2, Ph) were obtained by photolysis of the amines III. Photolysis of III (R = Ph) also yielded N-(3-hydroxyphthalimidinomethyl)phthalimide.
IT **56097-22-4P 56097-25-7P 56097-29-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 56097-22-4 HCAPLUS
CN 6H,13H,15H-Isoindolo[2'',1'':3',4']imidazo[5',1':2,3]imidazo[5,1-a]isoindole-6,15-dione, 4b,4c,10b,11-tetrahydro-4b,10b-dihydroxy- (9CI) (CA INDEX NAME)

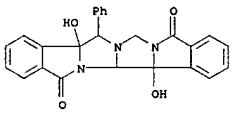


RN 56097-25-7 HCAPLUS
CN 6H,13H,15H-Isoindolo[2'',1'':3',4']imidazo[5',1':2,3]imidazo[5,1-a]isoindole-6,15-dione, 4b,4c,10b,11-tetrahydro-4b,10b-dihydroxy-11-(1-methylethyl)- (9CI) (CA INDEX NAME)



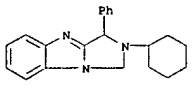
RN 56097-29-1 HCAPLUS
CN 6H,13H,15H-Isoindolo[2'',1'':3',4']imidazo[5',1':2,3]imidazo[5,1-a]isoindole-6,15-dione,
4b,4c,10b,11-tetrahydro-4b,10b-dihydroxy-11-phenyl- (9CI) (CA INDEX NAME)

L69 ANSWER 50 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

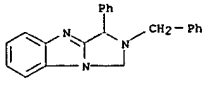


L69 ANSWER 51 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1974:520538 HCAPLUS
DOCUMENT NUMBER: 81:120538
TITLE: Syntheses of imidazo[1,5-a]- and pyrazino[1,2-b]benzimidazoles
AUTHOR(S): Schubert, H.; Lettau, H.; Fischer, J.
CORPORATE SOURCE: Sekt. Chem., Martin Luther Univ., Halle, Ger. Dem. Rep.
SOURCE: Tetrahedron (1974), 30(10), 1231-6
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 81:120538
GI For diagram(s), see printed CA Issue.
AB 2-(α-Chlorobenzyl)benzimidazolium chloride with R1NH2 gave the 2-(α-aminobenzyl)benzimidazoles I (R1 = H, cyclohexyl, CH2Ph, alkyl, aryl). The benzhydryl analogs (II) were prepared similarly. 1,2-Dihydro-3H-imidazo [1,5-a] benzimidazoles (III), 1-oxo-1,2-dihydro-3H-imidazo [1,5-a] benzimidazoles, 3-oxo-1,2,3,4-tetrahydropyrazino [1,2-a] benzimidazoles (IV), and 3,4-dioxo-1,2,3,4-tetrahydropyrazino [1,2-a] benzimidazoles were prepared by reaction of I and II with CH2O, COCl2, ClCHR2COCl, and (COCl)2, resp. II (R1 = H) with HC(OEt)3 gave 3,3-diphenyl-3H-imidazo[1,5-a] benzimidazole.
IT **54463-11-5P 54463-12-6P 54463-13-7P**
54463-14-8P 54463-15-9P 54463-17-1P
54463-18-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54463-11-5 HCAPLUS
CN 1H-Imidazo[1,5-a]benzimidazole, 2-cyclohexyl-2,3-dihydro-3-phenyl- (9CI) (CA INDEX NAME)

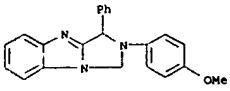


RN 54463-12-6 HCAPLUS
CN 1H-Imidazo[1,5-a]benzimidazole, 2,3-dihydro-3-phenyl-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

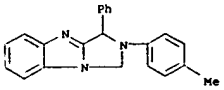


RN 54463-13-7 HCAPLUS
CN 1H-Imidazo[1,5-a]benzimidazole, 2,3-dihydro-2-(4-methoxyphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

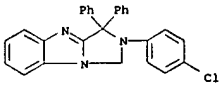
L69 ANSWER 51 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



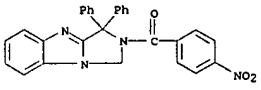
RN 54463-14-8 HCAPLUS
CN 1H-Imidazo[1,5-a]benzimidazole, 2,3-dihydro-2-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 54463-15-9 HCAPLUS
CN 1H-Imidazo[1,5-a]benzimidazole, 2-(4-chlorophenyl)-2,3-dihydro-3,3-diphenyl- (9CI) (CA INDEX NAME)

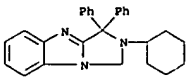


RN 54463-17-1 HCAPLUS
CN 1H-Imidazo[1,5-a]benzimidazole, 2,3-dihydro-2-(4-nitrobenzoyl)-3,3-diphenyl- (9CI) (CA INDEX NAME)



RN 54463-18-2 HCAPLUS
CN 1H-Imidazo[1,5-a]benzimidazole, 2-cyclohexyl-2,3-dihydro-3,3-diphenyl- (9CI) (CA INDEX NAME)

L69 ANSWER 51 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

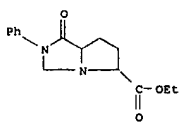


L69 ANSWER 52 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1974:437548 HCAPLUS
DOCUMENT NUMBER:	81:37548
TITLE:	Ethyl 1-oxoperhydropyrrolo [1,2-c] imidazolecarboxylates
INVENTOR(S):	Fontanella, Luigi; Occelli, Emilio
PATENT ASSIGNEE(S):	Gruppo Lepetit S.p.A.
SOURCE:	Ger. Offen., 12 pp. CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2354071	A1	19740516	DE 1973-2354071	19731029
GB 1381474	A	19750122	GB 1973-45809	19731001
US 3901911	A	19750826	US 1973-409985	19731026
FR 2205320	A1	19740531	FR 1973-38682	19731030
JP 49076893	A2	19740724	JP 1973-123938	19731102
PRIORITY APPLN. INFO.:			IT 1972-31275 A	19721103

GI For diagram(s), see printed CA Issue.
AB Ten esters [I; R = Me, Ph, C6H4OMe-4, or CH2Ph; R1 = Pr, Ph, or C6H3(OMe)2-3,4], useful as anxiolytics, hypnotics, muscle relaxants, or sedatives, were prepared by reaction of the pyrrolidines II with R1CHO in the presence of 4-MeC6H4SO3H in xylene at reflux, optionally followed by chromatog. separation into isomers.
IT **52840-79-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 52840-79-6 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-5-carboxylic acid, hexahydro-1-oxo-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

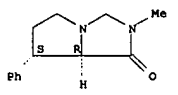


L69 ANSWER 53 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1974:425642 HCAPLUS
DOCUMENT NUMBER:	81:25642
TITLE:	Synthesis of aryl-substituted 1,3- and 1,4-diazocine derivatives
AUTHOR(S):	Sarges, Reinhard; Tretter, James R.
CORPORATE SOURCE:	Cent. Res., Pfizer Inc., Groton, CT, USA
SOURCE:	Journal of Organic Chemistry (1974), 39(12), 1710-16 CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 81:25642

GI For diagram(s), see printed CA Issue.
AB The synthesis of aryl-substituted 1,3- and 1,4-diazocine derivs. was undertaken because their structural features suggested potential central nervous system activity. Reaction of Me β-(bromomethyl)cinnamate with N,N'-dimethylethylene-diamine gave Me N,N'-dimethyl-2-phenylpiperazine-2-acetate which was converted to 1,4-dimethyl-7-phenyl-1,2,3,4-tetrahydro-1,4-diazocin-5(8H)-one (I). Catalytic and hydride reduction of I led ultimately to the 6-phenylperhydro-1,4-diazocine (II). Conversion of trans-3-phenylproline to III followed by desulfurization and quaternization with MeI gave the bicyclic intermediate IV, which on treatment with NaH or Li-NH3 underwent transannular ring opening to give 1,3-dimethyl-6-phenyl-1,2,3,7-tetrahydro-1,3-diazocin-4(8H)-one (V) and its perhydro analog, resp. Reaction of IV with NaOMe or with NaBH4 led to peripheral ring cleavage giving N-methyl-3-phenylproline methyl ester and the corresponding alc., resp.
IT **51212-44-3P 51212-45-4P 51212-46-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 51212-44-3 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-7-phenyl-, cis- (9CI) (CA INDEX NAME)

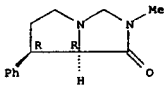
Relative stereochemistry.



RN 51212-45-4 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-7-phenyl-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

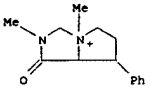
Relative stereochemistry.

L69 ANSWER 53 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● HCl

RN 51212-46-5 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazolium, hexahydro-2,4-dimethyl-1-oxo-7-phenyl-, iodide, trans- (9CI) (CA INDEX NAME)



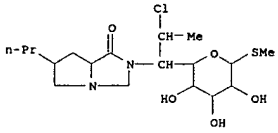
● I⁻

L69 ANSWER 54 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1973:515852 HCAPLUS
DOCUMENT NUMBER: 79:115852
TITLE: Lincomycin-type compounds
INVENTOR(S): Argoudelis, Alexander D.; Magerlein, Barney J.
PATENT ASSIGNEE(S): Upjohn Co.
SOURCE: U.S., 17 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

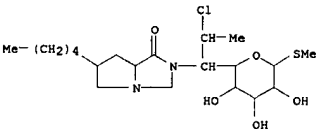
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3758454	A	19730911	US 1971-123891	19710312
JP 56047193	B4	19811107	JP 1972-24440	19720311
PRIORITY APPLN. INFO.:			US 1971-123891 A	19710312

GI For diagram(s), see printed CA Issue.
AB Treatment of 1'-demethyllincomycin derivs. with RCHO (R = e.g. H, 2-furyl p-BrC6H4) gave I (R = as above; R1, R2, = H, alkyl, R3 = halo, OH, OMe), useful as bactericides. Thus, 7(S)-chloro-7-deoxy-1'-demethyllincomycin-HCl reacted with HCHO in aqueous NaOH to give I [R = H, R1 = Me, R2 = Pr, R3 = Cl(S)]. Analogously, 7 more I were prepared Acetylation of Me 6,7-aziridino-6-deamino-7-deoxy-α-thiolincosaminide, followed by cleavage of the aziridine ring with HOAc at 130° and deacetylation gave Me 7-deoxy-7(S)-methoxy-α-thiolincosaminide (II).
IT **35119-67-6P 50613-38-2P 50613-39-3P 50613-40-6P 50613-43-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35119-67-6 HCAPLUS
CN L-threo-α-D-galacto-Octopyranoside, methyl 7-chloro-6,7,8-trideoxy-6-(tetrahydro-1-oxo-6-propyl-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1-thio-, (6R-cis)- (9CI) (CA INDEX NAME)

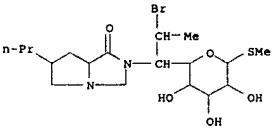


RN 50613-38-2 HCAPLUS
CN L-threo-α-D-galacto-Octopyranoside, methyl 7-chloro-6,7,8-trideoxy-6-(tetrahydro-1-oxo-6-pentyl-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1-thio-, [6(6R,7aS)]- (9CI) (CA INDEX NAME)

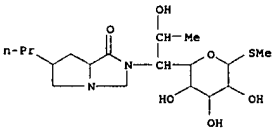
L69 ANSWER 54 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 50613-39-3 HCAPLUS
CN L-threo-α-D-galacto-Octopyranoside, methyl 7-bromo-6,7,8-trideoxy-6-(tetrahydro-1-oxo-6-propyl-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1-thio-, [6(6R,7aS)]- (9CI) (CA INDEX NAME)



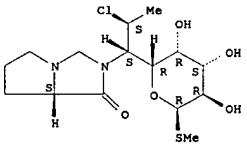
RN 50613-40-6 HCAPLUS
CN D-erythro-α-D-galacto-Octopyranoside, methyl 6,8-dideoxy-6-(tetrahydro-1-oxo-6-propyl-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1-thio-, [6(6R,7aS)]- (9CI) (CA INDEX NAME)



RN 50613-43-9 HCAPLUS
CN L-threo-α-D-galacto-Octopyranoside, methyl 7-chloro-6,7,8-trideoxy-6-(tetrahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1-thio-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

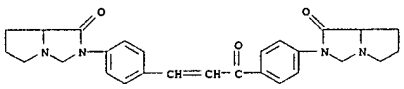
L69 ANSWER 54 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L69 ANSWER 55 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:147966 HCAPLUS
DOCUMENT NUMBER: 78:147966
TITLE: Chalcone derivatives
INVENTOR(S): Oshiro, Susumu; Nagura, Takeo; Sugihara, Yukio; Okamoto, Koji; Ishida, Ryuichi; Shintomi, Keiichi
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 48019595	B4	19730312	JP 1971-55101	19710722
JP 49032871		19740000	JP	

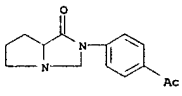
GI For diagram(s), see printed CA Issue.
AB Thetitle compds. (I), antispasmodics and tranquilizers, were prepared by the reaction of 1-oxopyrrolidinoimidazolidinyl-acylophenones with 1-oxopyrrolidinoimidazolidinylbenzaldehydes. E.g., 9.8 g p-(1-oxopyrrolidino[1,2-c]imidazolidin-2-yl)propiophenone an 9.3 g p-(1-oxopyrrolidino[1,2-c]imidazolidin-2-yl)-benzaldehyde in MeOH was heated 5 hr at 40-50° with 20% NaOH solution to give 72% I (R1 = R3 = H, R2 = Me). Similarly prepared were I.2HCl (R1, R2, R3 and % yield given):
Me, H, H, 58.5%; H, H, H, -; H, h, Me, 77.
IT **41038-71-5P 41124-24-7P 41124-25-8P 41373-84-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 41038-71-5 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-[4-[1-oxo-3-[4-(tetrahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)phenyl]-2-propenyl]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



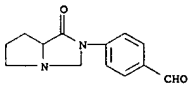
●2 HCl

RN 41124-24-7 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2,2'-[(2-methyl-3-oxo-1-propene-1,3-diyl)di-4,1-phenylene]bis[hexahydro- (9CI) (CA INDEX NAME)

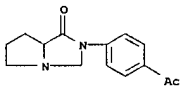
L69 ANSWER 55 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



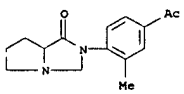
RN 41373-86-8 HCAPLUS
CN Benzaldehyde, 4-(tetrahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)- (9CI) (CA INDEX NAME)



IT **32901-73-8 41373-89-1 41518-30-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzaldehydes)
RN 32901-73-8 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-acetylphenyl)hexahydro- (9CI) (CA INDEX NAME)

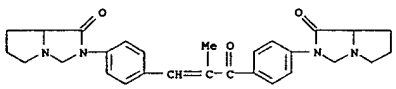


RN 41373-89-1 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-acetyl-2-methylphenyl)hexahydro- (9CI) (CA INDEX NAME)

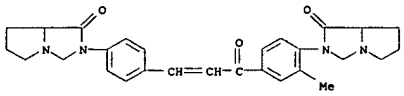


RN 41518-30-3 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-[4-(1-oxopropyl)phenyl]- (9CI) (CA INDEX NAME)

L69 ANSWER 55 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

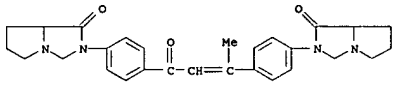


RN 41124-25-8 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-[4-[3-[3-methyl-4-(tetrahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)phenyl]-3-oxo-1-propenyl]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

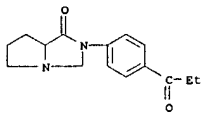
RN 41373-84-6 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2,2'-[(1-methyl-3-oxo-1-propene-1,3-diyl)di-4,1-phenylene]bis[hexahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

IT **32901-73-8 41373-86-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetophenones)
RN 32901-73-8 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-acetylphenyl)hexahydro- (9CI) (CA INDEX NAME)

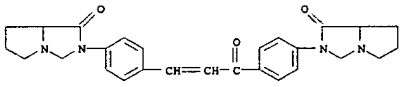
L69 ANSWER 55 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L69 ANSWER 56 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:147963 HCAPLUS
DOCUMENT NUMBER: 78:147963
TITLE: Chalcone derivatives
INVENTOR(S): Oshiro, Susumu; Nagura, Takeo; Sugihara, Yukio; Okamoto, Koji; Ishida, Ryuichi; Shintomi, Keiichi
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 48019594	B4	19730312	JP 1971-55100	19710722
JP 49032870		19740326	JP 1972-74874	19720726

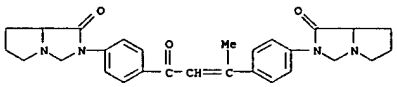
GI For diagram(s), see printed CA Issue.
AB The title compds. (I), antispasmodics and tranquilizers, were prepared by treating 4,4'-diprolylaminochalcones with HCHO or with N,N'-carbonyldiimidazole (carbonalating agent). E.g., 18.5 g 4,4'-bis(L-prolylamino)-β-methylchalcone in MeOH was stirred 5 hr at 50° with 13.4 g 37% HCHO to give 97% I (X = CH2, R1 = Me, R2 = R3 = H). Similarly prepared were the following I (X, R1, R2, R3, and % yield given): CH2, H, Me, H, 85; CH2, H, H, H, 72% (dihydrochloride); CH2, H, H, Me, 82 (dihydrochloride); CO, Me, H, H, 45.
IT **41038-71-5P 41124-23-6P 41124-24-7P 41124-25-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 41038-71-5 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-[4-[1-oxo-3-[4-(tetrahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)phenyl]-2-propenyl]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



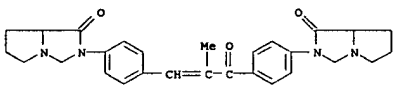
●2 HCl

RN 41124-23-6 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2,2'-[(1-methyl-3-oxo-1-propene-1,3-diyl)di-4,1-phenylene]bis[hexahydro- (9CI) (CA INDEX NAME)

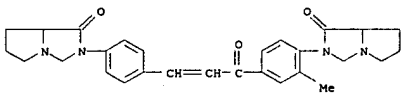
L69 ANSWER 56 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 41124-24-7 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2,2'-[(2-methyl-3-oxo-1-propene-1,3-diyl)di-4,1-phenylene]bis[hexahydro- (9CI) (CA INDEX NAME)

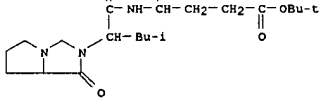


RN 41124-25-8 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-[4-[3-[3-methyl-4-(tetrahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)phenyl]-3-oxo-1-propenyl]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



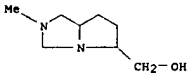
●2 HCl

L69 ANSWER 57 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:97999 HCAPLUS
DOCUMENT NUMBER: 78:97999
TITLE: N,N'-alkylidene peptides. Peptide synthesis by products in the action of carbonyl compounds
AUTHOR(S): Cardinaux, F.; Brenner, M.
CORPORATE SOURCE: Inst. Org. Chem., Univ. Basel, Basel, Switz.
SOURCE: Helvetica Chimica Acta (1973), 56(1), 339-47
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Hydrogenolysis of Z-Pro-Leu-Glu(OCMe3)-Phe-OCMe3, Z-Val-His-Pro-PHeOMe, and Z-Val-Tyr-Val-His-Pro-PHeOMe (Z = PhCH2OC) yields by-products that were identified as 4-imidazolidinone derivs. They were formed by cycloaddn. of a carbonyl compound, formed by oxidation of the solvent under the reaction conditions, to the newly liberated N-terminal of the peptide and to the N of the adjacent amino acid residue.
IT **40149-18-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40149-18-6 HCAPLUS
CN L-Phenylalanine, N-[N-[4-methyl-1-oxo-2-(tetrahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)pentyl]-L-α-glutaminyl]-, bis(1,1-dimethylethyl) ester, stereoisomer (9CI) (CA INDEX NAME)

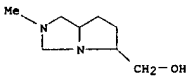


L69 ANSWER 58 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:429613 HCAPLUS
DOCUMENT NUMBER: 77:29613
TITLE: Microbial transformation of antibiotics. VII. Hydroxymethylation of N-demethylclindamycin
AUTHOR(S): Argoudelis, A. D.; Coats, J. H.; Magerlein, B. J.
CORPORATE SOURCE: Res. Lab., Upjohn Co., Kalamazoo, MI, USA
SOURCE: Journal of Antibiotics (1972), 25(3), 191-3
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
AB N-demethylclindamycin (I) [22431-45-4] was hydroxymethylated by Streptomyces lincolnensis to yield N-demethyl-N-hydroxymethylclindamycin (II) [35155-31-8], which was subsequently dehydrated under the fermentation conditions to yield the bicyclic imidazolidone, 2-[7-chloro-1,6,7,8-tetradeoxy-1α-(methylthio)-L-threo-D-galacto-6-octapyranosyl]hexahydro-6-propyl-1H-pyrrolo[1,2-c]imidazol-1-one (III) [**35119-67-6**].
IT **35119-67-6**
RL: FORM (Formation, nonpreparative)
(formation of, from demethylclindamycin by Streptomyces lincolnensis)
RN 35119-67-6 HCAPLUS
CN L-threo-α-D-galacto-Octopyranoside, methyl 7-chloro-6,7,8-trideoxy-6-(tetrahydro-1-oxo-6-propyl-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-1-thio-, (6R-cis)- (9CI) (CA INDEX NAME)

L69 ANSWER 59 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1971:488591 HCAPLUS
DOCUMENT NUMBER: 75:88591
TITLE: 5-Oxa-3,10-diazabicyclo[5.2.1]decane and 5-oxa-3,10-diazabicyclo[5.2.1]decan-4-one derivatives, potentially active on the central nervous system
AUTHOR(S): Fontanella, L.; Occelli, E.
CORPORATE SOURCE: Lab. Ric., Gruppo Lepetit S.p.A., Milan, Italy
SOURCE: Farmaco, Edizione Scientifica (1971), 26(8), 685-709
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: Italian
OTHER SOURCE(S): CASREACT 75:88591
GI For diagram(s), see printed CA Issue.
AB 3,10-Diethyl-5-oxa-3,10-diazabicyclo[5.2.1] decane (I) and II are prepared from III. Thus, III (R = R1 = Et) is treated with H2CO to give I. III (R = R1 = Me) is treated with COCl2 and KOH to give II (R = Me). Similarly prepared are 9 other II (R = C3-4 alkyl, PhCH2, Ph, (CH2)2NMe2, aralkyl, or substituted phenyl).
IT **33252-12-9P 33252-13-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 33252-12-9 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-5-methanol, hexahydro-2-methyl- (8CI) (CA INDEX NAME)



RN 33252-13-0 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-5-methanol, hexahydro-2-methyl-, dihydrochloride (8CI) (CA INDEX NAME)



●2 HCl

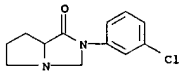
L69 ANSWER 59 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L69 ANSWER 60 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1971:449087 HCAPLUS
DOCUMENT NUMBER: 75:49087
TITLE: Pyrrolidino[1,2-c]imidazolidinone derivatives
INVENTOR(S): Oshiro, Susumu; Nakura, Takeo; Okamoto, Takashi; Okumura, Kentaro
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd.
SOURCE: Jpn. Tokkyo Koho, 4 pp.
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 46016990	B4	19710511	JP	19680319

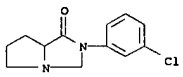
GI For diagram(s), see printed CA Issue.
AB I, useful as anti-inflammatory, analgesic, and antispasmodic drugs, are manufactured by reaction of II with R2CHO. II (R2 = Ph) (11.5 g) in 50 ml MeOH is stirred 3 hr with 7.4 g 37% HCHO to give 11.7 g I (R1 = Ph, R2 = H), m. 63-5°, hydrochloride m. 203° (decomposition). Similarly prepared are I (R1, R2, m.p., and that of the hydrochloride given): 3-ClC6H4, H, 107-8°, 184°; 4-MeOC6H4, H 113-15°, 175-6°; Ph, Me, 90°, 151°; Ph, PhCH2, 135-7°, 179°; Ph, 2-furyl, 173-5°, 163-5; 2-methyl-6-pyridyl, H, -(oil), 163-5°; Pr, H, -(oil), 157-9°; Bu, H, -(oil), 145-7°; PhCH2, H, -(oil), 169-71°; 2-ClC6H4, H, -(oil), 198-9°; 4-ClC6H4, H, 95-6°, 141-3°; 2-MeOC6H4, H,-(oil), 193-5°; 3-NO2C6H4, H, 141-3°, 196°; 4-NO2C6H4, H, 198-200°, 174-6°; 4-H2NSO2C6H4, H, 300°,-; 3-H2NC6H4, H, -, 275°; 4-AcC6H4, H, 174-6°, 300°; Ph, Et, -(oil), 166-8°; Ph, Ph, 138-9°, 190-1°; Ph, iso-Pr, 130°, 152-4°; Ph, 2-HOC6H4, 89-91°, 188-90°; Ph, 3-MeOC6H4, 117-19°, 226-8°; Ph, 3-HOC6H4, 117-19°.-.
IT **32901-46-5P 32901-47-6P 32901-48-7P 32901-49-8P 32901-55-6P 32901-56-7P 32901-57-8P 32901-58-9P 32901-59-0P 32901-60-3P 32901-61-4P 32901-62-5P 32901-63-6P 32901-64-7P 32901-65-8P 32901-66-9P 32901-67-0P 32901-68-1P 32901-69-2P 32901-70-5P 32901-71-6P 32901-72-7P 32901-73-8P 32901-74-9P 32902-37-7P 32902-38-8P 33035-95-9P 34062-99-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 32901-46-5 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(m-chlorophenyl)hexahydro-, monohydrochloride (8CI) (CA INDEX NAME)

L69 ANSWER 60 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

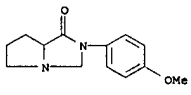


● HCl

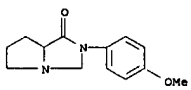
RN 32901-47-6 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(m-chlorophenyl)hexahydro- (8CI) (CA INDEX NAME)



RN 32901-48-7 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(p-methoxyphenyl)- (8CI) (CA INDEX NAME)



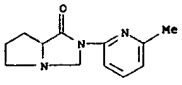
RN 32901-49-8 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(p-methoxyphenyl)-, monohydrochloride (8CI) (CA INDEX NAME)



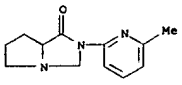
● HCl

RN 32901-55-6 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(6-methyl-2-pyridyl)- (8CI) (CA INDEX NAME)

L69 ANSWER 60 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

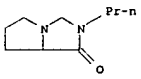


RN 32901-56-7 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(6-methyl-2-pyridyl)-, monohydrochloride (8CI) (CA INDEX NAME)

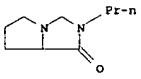


● HCl

RN 32901-57-8 HCAPLUS
CN 1H-Pyrrolo]1,2-c]imidazol-1-one, hexahydro-2-propyl- (8CI) (CA INDEX NAME)



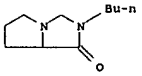
RN 32901-58-9 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-propyl-, monohydrochloride (8CI) (CA INDEX NAME)



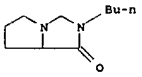
● HCl

RN 32901-59-0 HCAPLUS

L69 ANSWER 60 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-butylhexahydro- (8CI) (CA INDEX NAME)

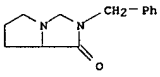


RN 32901-60-3 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-butylhexahydro-, monohydrochloride (8CI) (CA INDEX NAME)

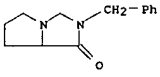


● HCl

RN 32901-61-4 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-benzylhexahydro- (8CI) (CA INDEX NAME)



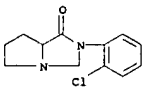
RN 32901-62-5 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-benzylhexahydro-, monohydrochloride (8CI) (CA INDEX NAME)



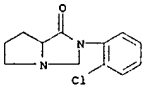
● HCl

RN 32901-63-6 HCAPLUS

L69 ANSWER 60 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(o-chlorophenyl)hexahydro- (8CI) (CA INDEX NAME)

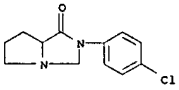


RN 32901-64-7 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(o-chlorophenyl)hexahydro-, monohydrochloride (8CI) (CA INDEX NAME)

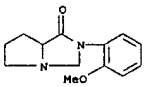


● HCl

RN 32901-65-8 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(p-chlorophenyl)hexahydro- (8CI) (CA INDEX NAME)

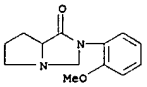


RN 32901-66-9 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(o-methoxyphenyl)- (8CI) (CA INDEX NAME)



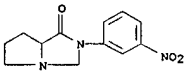
RN 32901-67-0 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(o-methoxyphenyl)-, monohydrochloride (8CI) (CA INDEX NAME)

L69 ANSWER 60 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

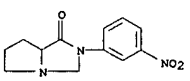


● HCl

RN 32901-68-1 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(m-nitrophenyl)- (8CI) (CA INDEX NAME)

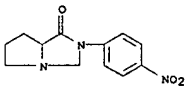


RN 32901-69-2 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(m-nitrophenyl)-, monohydrochloride (8CI) (CA INDEX NAME)



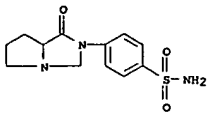
● HCl

RN 32901-70-5 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(p-nitrophenyl)- (8CI) (CA INDEX NAME)

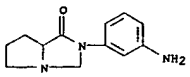


RN 32901-71-6 HCAPLUS
CN Benzenesulfonamide, p-(tetrahydro-1-oxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)- (8CI) (CA INDEX NAME)

L69 ANSWER 60 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

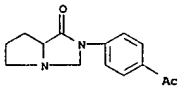


RN 32901-72-7 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(m-aminophenyl)hexahydro-, monohydrochloride (8CI) (CA INDEX NAME)



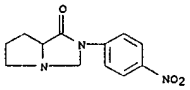
● HCl

RN 32901-73-8 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-acetylphenyl)hexahydro- (9CI) (CA INDEX NAME)



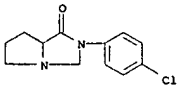
RN 32901-74-9 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(p-acetylphenyl)hexahydro-, monohydrochloride (8CI) (CA INDEX NAME)

L69 ANSWER 60 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



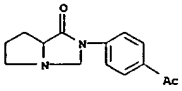
● HCl

RN 34062-99-2 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(p-chlorophenyl)hexahydro-, monohydrochloride (8CI) (CA INDEX NAME)



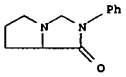
● HCl

L69 ANSWER 60 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

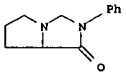


● HCl

RN 32902-37-7 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl- (8CI) (CA INDEX NAME)



RN 32902-38-8 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-, monohydrochloride (8CI) (CA INDEX NAME)



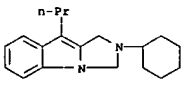
● HCl

RN 33035-95-9 HCAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(p-nitrophenyl)-, monohydrochloride (8CI) (CA INDEX NAME)

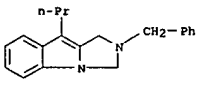
L69 ANSWER 61 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1971:76254 HCAPLUS
DOCUMENT NUMBER: 74:76254
TITLE: Reaction of 3-propylindole with aldehydes. Preparation of 2-(α-aminoalkyl)indoles
AUTHOR(S): Wolinsky, Joseph; Sundeen, J. E.
CORPORATE SOURCE: Dep. Chem., Purdue Univ., Lafayette, IN, USA
SOURCE: Tetrahedron (1970), 26(23), 5427-35
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 74:76254
GI For diagram(s), see printed CA Issue.
AB 2,2'-Benzylidenebisindoles (I) are produced by the condensation of 3-propylindole with aromatic aldehydes. Aromatic aldehydes react initially, but reversibly, at N. N-Substituted products can be trapped as acetate derivs. and are converted to I under the original reaction conditions. 3-Propylindole reacts with HCHO and piperidine under mild conditions to give 1-piperidinomethyl-3-propylindole. 2-Piperidinomethyl-3-propylindole is obtained when the reaction with HCHO in AcOH is carried out at 100° in the presence of excess piperidine. The condensation of 3-propylindole with HCHO and primary amines, such as PhCH2NH2, involves initial attack at N followed by intramol. substitution at the 2-position to yield 2-benzyl-2,3-dihydro-9-propyl-1H-imidazo-[1,5-a]indole (II) and 2,4-dibenzyl-11-propyl-2,3,4,5-tetrahydro-1,3,5-triazepino[1,7-a]indole (III). Hydrolysis of cyclohexyl-imidazoindole affords 2-cyclohexylaminomethyl-3-propylindole.
IT **30713-07-6P**, 1H-Imidazo[1,5-a]indole, 2-cyclohexyl-2,3-dihydro-9-propyl- **30745-26-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 30713-07-6 HCAPLUS
CN 1H-Imidazo[1,5-a]indole, 2-cyclohexyl-2,3-dihydro-9-propyl- (9CI) (CA INDEX NAME)

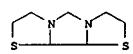


RN 30745-26-7 HCAPLUS
CN 1H-Imidazo[1,5-a]indole, 2-benzyl-2,3-dihydro-9-propyl- (8CI) (CA INDEX NAME)

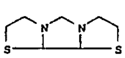


L69 ANSWER 61 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L69 ANSWER 62 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1968:467279 HCAPLUS
DOCUMENT NUMBER: 69:67279
TITLE: Thiazolidine. I. Formation and reactions of 3,3'-methylenedithiazolidine
AUTHOR(S): Takatori, Toshisuke; Kojima, Masaharu; Taguchi, Tanezo
CORPORATE SOURCE: Kyushu Univ., Fukuoka, Japan
SOURCE: Yakugaku Zasshi (1968), 88(3), 360-5
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI For diagram(s), see printed CA Issue.
AB 2-Aminoethanethiol (3 g.) in 12 ml. H2O is treated with 3.5 ml. 37% formalin to give 3.1 g. 3,3'-methylenedithiazolidine (I) (n = 0), m. 48-9° (petroleum ether). Similarly is prepared dl-3,3'-methylenebis(perhydrocyclohexa[d]thiazole) (I) (n = 4); trans isomer m. 97-8°; cis isomer m. 101-2°. trans-2-Aminocyclohexanethiol (2 g.) in 10 ml. H2O is treated with 2 ml. AcOH to give 1.5 g. trans-II (R1 = Me, R2 = H), m. 50-1°; HCl salt m. 173-4°. Similarly prepared are the following trans-II (R1, R2, m.p., and m.p. HCl salt given): Me, Me, - (b8 89-90°), 53-4°; Ph, H, 53-4°, 193-5°; and (R1R2 =) (CH2)5, -, 35-6°, 225-7°. Warming 2 g. 2,2'dithiazolidine in 10 ml. H2O with 2 ml. 37% formalin gives perhydroimidazo[1,5-b;4,3-b']dithiazole (III), m. 80-1° (petroleum ether). I (n = 0) (5.0 g.) and 3.0 g. PhOH is stirred 24 hrs. in 20 ml. Et2O at room temperature, evaporated, and the residue in 1:1 petroleum ether-C6H6 chromatographed on 120 g. SiO2 to give 3.1 g. 3-(o-hydroxybenzyl)thiazolidine, m. 73.5-4.5° (petroleum ether). The use of PhCH2SH instead of PhOH in the above reaction gives 3-(benzylthiomethyl)thiazolidine, m. 88-90° (EtOH).
IT 19505-80-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19505-80-7 HCAPLUS
CN 5H-Imidazo[5,1-b:4,3-b']bisthiazole, hexahydro- (7CI, 8CI) (CA INDEX NAME)



L69 ANSWER 63 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:27236 HCAPLUS
DOCUMENT NUMBER: 58:27236
ORIGINAL REFERENCE NO.: 58:4536b-e
TITLE: A new development in the formation reaction of thiazolidines from 2-arminoalkanethiols and carbonyl compounds
AUTHOR(S): Taguchi, Tanezo; Takatori, Toshisuke; Kojima, Masaharu
CORPORATE SOURCE: Kyushu Univ., Fukuoka
SOURCE: Chemical & Pharmaceutical Bulletin (1962), 10, 245-6
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 58:27236
AB HSCH2CH2NH2 (I) treated with HCHO gave bis(3-thiazolidinyl) methane (II), m. 48-9°, which set free HCHO and gave the HCl salt (III) of thiazolidine (IV) with HCl-EtOH. The structure of II was confirmed by its infrared (I.R.) spectrum, and by its formation from IV with HCHO. I with other carbonyl compds. gave the corresponding simple thiazolidines, which did not give analogs of II with HCHO. 2,2'-Dithiazolidine with HCHO gave perhydroimidazo[1,5-b:4,3-b']dithiazole (V), m. 80-1°, confirmed by its I.R. spectrum. Similar treatment of the HCl salts of cis- and trans-aminocyclohexanethiols (VI) with HCHO gave cis- and trans-cyclohexa[d]thiazolidine-HCl (VII), m. 204-5° and 211-12°, resp., whereas free VI (like free I) gave analogs of II, cis- and trans-3,3'-methylenebis[cyclohexa[d]thiazolidine], m. 101-2°, and 97-8°, resp., which, like II, freed HCHO and gave VII with HCl-EtOH. VI with D-glucose gave [by analogy with the products from I with D-glucose (Bonner and Meyer, CA 55, 13412b)] 2-(D-gluco-1,2,3,4,5-pentahydroxypentyl)(-)-cis- and (-)-trans-cyclohexa[d]thiazolidine (VIII), m. 152-3°, [α]17D -61.4°, and 161-3°, [α]17D 15.6°, resp. Boiling VIII with cyclohexanone exchanged the D-glucose group for the cyclohexane ring to give (-)-cis- and (+)-trans-spiro[cyclohexane-1,2'-cyclohexa[d]thiazolidine] (IX), HCl salts m. 228-30° ([α]17D -65.6°) and 229-31° ([α]17D 65.6°), resp. IX were hydrolyzed with HCl to give (-)-cis- and (+)-trans-2-aminocyclohexanethiol-HCl, m. 217-19° ([α]17D -49.1°) and 215-17° ([α]17D 49.0°), resp. Thus, a new method of optical resolution was made available for other resolvable aminoalkanethiols and aminoalkanols.
IT 19505-80-7, 5H-Imidazo[5,1-b:4,3-b']bisthiazole, hexahydro-
(preparation of)
RN 19505-80-7 HCAPLUS
CN 5H-Imidazo[5,1-b:4,3-b']bisthiazole, hexahydro- (7CI, 8CI) (CA INDEX NAME)



L69 ANSWER 63 OF 63 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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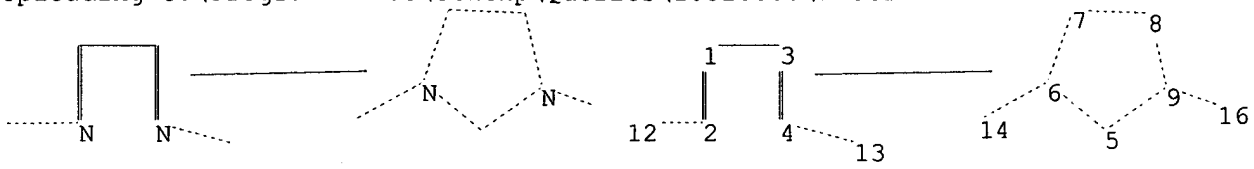


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ring nodes :
5  6  7  8  9
ring/chain nodes :
1  2  3  4  12  13  14  16
ring/chain bonds :
1-2  1-3  2-12  3-4  4-13  6-14  9-16
ring bonds :
5-6  5-9  6-7  7-8  8-9
exact/norm bonds :
1-2  1-3  2-12  3-4  4-13  5-6  5-9  6-7  6-14  7-8  8-9  9-16


Connectivity :
2:2 E exact RC ring/chain  4:2 E exact RC ring/chain  5:2 E exact RC ring/chain
Match level :
1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom
12:CLASS  13:CLASS  14:CLASS  16:CLASS
fragments assigned product role:
containing 5
fragments assigned reactant/reagent role:
containing 1
node mappings:
2:6  1:7  3:8  4:9  12:14  13:16



L60     STRUCTURE UPLOADED

=> s L60
SAMPLE SEARCH INITIATED 12:16:23 FILE 'CASREACT'
SCREENING COMPLETE -   7817 REACTIONS TO VERIFY FROM      611 DOCUMENTS

 64.0% DONE    5000 VERIFIED       2 HIT RXNS                        1 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:    151073 TO   161607
PROJECTED ANSWERS:               1 TO      141

L61           1 SEA SSS SAM L60 (     2 REACTIONS)

=> s L60 full
FULL SEARCH INITIATED 12:16:30 FILE 'CASREACT'
SCREENING COMPLETE - 169853 REACTIONS TO VERIFY FROM    12466 DOCUMENTS
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100.0% DONE 169853 VERIFIED 111 HIT RXNS (3 INCOMP) 35 DOCS
SEARCH TIME: 00.00.02

L62 35 SEA SSS FUL L60 (111 REACTIONS)

=> d sca

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=>  file casreact
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    332.05    1388.13

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -47.25     -47.25

FILE 'CASREACT' ENTERED AT 12:29:25 ON 28 JUN 2006
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FILE CONTENT:1840 - 25 Jun 2006 VOL 144 ISS 26

New CAS Information Use Policies, enter HELP USAGETERMS for details.

************************************************************
*                                                          *
*     CASREACT now has more than 10 million reactions      *
*                                                          *
************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> d his

     (FILE 'HOME' ENTERED AT 09:32:44 ON 28 JUN 2006)

     FILE 'REGISTRY' ENTERED AT 09:32:52 ON 28 JUN 2006
L1      1650308 S NCNC2/ESS

     FILE 'REGISTRY' ENTERED AT 09:51:45 ON 28 JUN 2006
L2              STRUCTURE UPLOADED
L3           8980 S L2 FULL
L4              STRUCTURE UPLOADED
L5           3519 S L4 FULL
L6             50 S L4
L7             50 S L2
                SAVE TEMP L5 GLOR800STR2/A

     FILE 'HCAPLUS' ENTERED AT 10:08:22 ON 28 JUN 2006
L8            253 S L5

     FILE 'REGISTRY' ENTERED AT 10:08:52 ON 28 JUN 2006
L9            628 S NC>1 AND L5
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     FILE 'STNGUIDE' ENTERED AT 10:12:24 ON 28 JUN 2006

     FILE 'REGISTRY' ENTERED AT 10:14:37 ON 28 JUN 2006
L10             STRUCTURE UPLOADED
L11          50 S L10 SAM SSS  SUB=L5
L12        1426 S L10 FULL SSS  SUB=L5

     FILE 'HCAPLUS' ENTERED AT 10:17:32 ON 28 JUN 2006
L13         108 S L12

     FILE 'REGISTRY' ENTERED AT 10:17:46 ON 28 JUN 2006
L14         237 S L12 AND NRRS>2

     FILE 'HCAPLUS' ENTERED AT 10:27:31 ON 28 JUN 2006
L15          56 S L14

     FILE 'REGISTRY' ENTERED AT 10:27:55 ON 28 JUN 2006
L16        1189 S L12 NOT L14

     FILE 'HCAPLUS' ENTERED AT 10:28:11 ON 28 JUN 2006
L17          60 S L16
L18           8 S L15 AND L17

     FILE 'REGISTRY' ENTERED AT 10:29:05 ON 28 JUN 2006

     FILE 'STNGUIDE' ENTERED AT 10:29:18 ON 28 JUN 2006

     FILE 'REGISTRY' ENTERED AT 10:45:47 ON 28 JUN 2006
L19             STRUCTURE UPLOADED
L20          32 S L19 SAM SSS  SUB=L12
L21         551 S L19 FULL SSS  SUB=L12

     FILE 'HCAPLUS' ENTERED AT 10:52:12 ON 28 JUN 2006
L22          85 S L21

     FILE 'REGISTRY' ENTERED AT 10:53:23 ON 28 JUN 2006
L23         368 S L21 NOT L14

     FILE 'HCAPLUS' ENTERED AT 10:53:51 ON 28 JUN 2006
L24          45 S L23

     FILE 'REGISTRY' ENTERED AT 10:54:25 ON 28 JUN 2006
L25         875 S L12 NOT L21
L26         821 S L12 NOT (L21 OR L14)
L27        3310 S 180.306.6/RID
L28         809 S L26 AND L27
L29          12 S L26 NOT L28

     FILE 'STNGUIDE' ENTERED AT 11:02:16 ON 28 JUN 2006

     FILE 'REGISTRY' ENTERED AT 11:04:38 ON 28 JUN 2006
L30             STRUCTURE UPLOADED
L31           1 S L30 SAM SSS  SUB=L12
L32          35 S L30 FULL SSS  SUB=L12
L33           0 S L32 AND L24
L34          35 S L32 AND L14
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     FILE 'HCAPLUS' ENTERED AT 11:07:03 ON 28 JUN 2006
L35           11 S L34

     FILE 'REGISTRY' ENTERED AT 11:07:31 ON 28 JUN 2006

     FILE 'HCAPLUS' ENTERED AT 11:08:14 ON 28 JUN 2006
L36           54 S L35 OR L24

     FILE 'REGISTRY' ENTERED AT 11:11:52 ON 28 JUN 2006
L37          403 S L23 OR L32

     FILE 'HCAPLUS' ENTERED AT 11:13:36 ON 28 JUN 2006
L38            1 S US2005-520800/APPS
                 SEL RN

     FILE 'REGISTRY' ENTERED AT 11:14:26 ON 28 JUN 2006
L39          109 S E1-E109
L40           34 S L39 AND L37
L41           75 S L39 NOT L40
L42            9 S L14 AND L39
L43          202 S L14 NOT L32

     FILE 'HCAPLUS' ENTERED AT 11:26:41 ON 28 JUN 2006
L44           47 S L43

     FILE 'REGISTRY' ENTERED AT 11:27:00 ON 28 JUN 2006

     FILE 'STNGUIDE' ENTERED AT 11:31:48 ON 28 JUN 2006

     FILE 'REGISTRY' ENTERED AT 11:35:19 ON 28 JUN 2006
L45              STRUCTURE UPLOADED
L46            2 S L45 SAM SSS  SUB=L12
L47           46 S L45 FULL SSS  SUB=L12
L48           46 S L14 AND L47

     FILE 'HCAPLUS' ENTERED AT 11:37:27 ON 28 JUN 2006
L49           12 S L48
L50           63 S L24 OR L35 OR L49

     FILE 'REGISTRY' ENTERED AT 11:38:49 ON 28 JUN 2006
L51          191 S L14 NOT L47
L52          161 S L14 NOT (L47 OR L32)

     FILE 'REGISTRY' ENTERED AT 11:52:20 ON 28 JUN 2006
                 SAVE TEMP L23 GLOR800L23/A
                 SAVE TEMP L34 GLOR800L34/A
                 SAVE TEMP L48 GLOR800L48/A

     FILE 'HCAPLUS' ENTERED AT 11:55:09 ON 28 JUN 2006
                 SAVE TEMP L50 GLOR800L50/A

     FILE 'CASREACT' ENTERED AT 12:03:57 ON 28 JUN 2006
L53              STRUCTURE UPLOADED
L54            1 S L53 SAM SSS
L55          113 S L53 FULL SSS
L56           85 S L55/COM
L57              STRUCTURE UPLOADED
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L58             1 S L57 SAM SSS
L59             8 S L57 FULL SSS
L60               STRUCTURE UPLOADED
L61             1 S L60
L62            35 S L60 FULL

     FILE 'HCAPLUS' ENTERED AT 12:20:00 ON 28 JUN 2006
L63            35 S L62
L64             3 S L50 AND L63
L65            24 S GLORIUS F?/AU
L66             6 S L65 AND L50
L67             4 S L65 AND L63
L68             3 S L66 AND L67
L69            63 S L66 OR L50

     FILE 'REGISTRY' ENTERED AT 12:26:44 ON 28 JUN 2006

     FILE 'HCAPLUS' ENTERED AT 12:26:50 ON 28 JUN 2006

     FILE 'CASREACT' ENTERED AT 12:29:25 ON 28 JUN 2006

=> d ibib abs hit L62 1-35
```

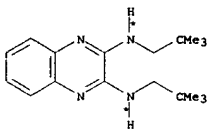
L62 ANSWER 1 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 144:350821 CASREACT
TITLE: Influence of annelation in N-heterocyclic carbenes: Novel quinoxaline-annelated NHCs trapped as transition metal complexes
AUTHOR(S): Saravanakumar, Shanmuganathan; Kindermann, Markus K.; Heinicke, Joachim; Koeckerling, Martin
CORPORATE SOURCE: Institut fuer Chemie und Biochemie, Ernst-Moritz-Arndt-Universitaet Greifswald, Greifswald, 17487, Germany
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2006), (6), 640-642
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

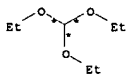
AB Quinoxaline-annelated imidazol-2-ylidenes are less stable in comparison to their non-annelated analogs, featuring high acidity of the C-H group of the parent quinoxalino[2,3-d]imidazolium salts; rhodium and silver complexes of the quinoxalino[2,3-d]imidazolylidenes were isolated and characterized. Orthoformate condensation with N,N'-R2-2,3-quinoxalinediamine gave 1,3-R2-quinoxalino[2,3-d]imidazolium hexafluorophosphates (2a,b; R = tBuCH2, iPr). Deprotonation of 2a by KH in the presence of [Rh(cod)Cl]2 gave the corresponding [(L-CH2tBu)Rh(cod)Cl] (L-CH2tBu = 1,3-dineopentylquinoxalino[2,3-d]imidazol-2-ylidene), whereas the free ligand L-CH2tBu (3) is unstable and non-detectable even at -50°. Metalation of 2b by Ag2O gave the cationic silver complex [(L-iPr)2Ag]PF6. The synthesis, NMR-, and crystal structure data of novel electron-deficient quinoxaline annelated imidazol-2-ylidene precursors and complexes thereof are reported and compared with related less electron-withdrawing or non-annelated N-heterocyclic carbenes and complexes to illustrate annelation effects.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 18 ...C + F ===> G...



C



F

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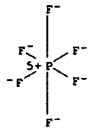
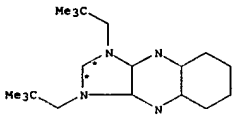


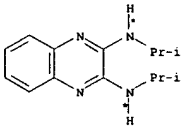
G: CM 1
YIELD 52%



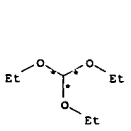
G: CM 2
YIELD 52%

RX(3) RCT C 881020-50-4, F 122-51-0
RGT H 16941-11-0 PF6.NH4
PRO G 881020-53-7
SOL 122-51-0 CH(OEt)3
CON 5 hours, 120 deg C

RX(4) OF 18 ...E + F ===> I...

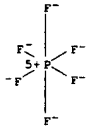


E

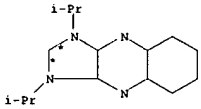


F

(4) →



I: CM 1
YIELD 76%

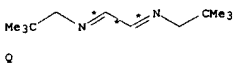


I: CM 2
YIELD 76%

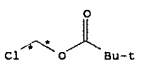
L62 ANSWER 1 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(4) RCT E 881020-51-5, F 122-51-0
RGT H 16941-11-0 PF6.NH4
PRO I 881020-55-9
SOL 122-51-0 CH(OEt)3
CON 24 hours, 120 deg C

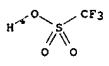
RX(7) OF 18 Q + R + S ===> T...



Q



R

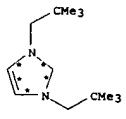


● Ag(I)

S

(7) →

T: CM 1
YIELD 72%

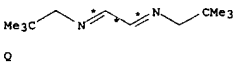


T: CM 2
YIELD 72%

RX(7) RCT Q 78198-90-0, R 18997-19-8, S 2923-28-6
PRO T 883990-73-6
SOL 75-09-2 CH2Cl2
CON 24 hours, 50 deg C
NTE in the dark

RX(9) OF 18 Q + R ===> V...

L62 ANSWER 1 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



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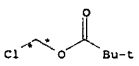
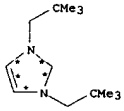


R

(9) →

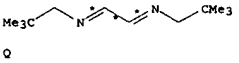
V: CM 1
YIELD 71%



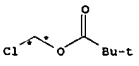
V: CM 2
YIELD 71%

RX(9) RCT Q 78198-90-0, R 18997-19-8
RGT W 14104-20-2 AgBF4
PRO V 881020-59-3
SOL 75-09-2 CH2Cl2
CON 24 hours, 50 deg C
NTE in the dark

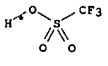
RX(15) OF 18 COMPOSED OF RX(7), RX(8)
RX(15) Q + R + S ===> U



Q



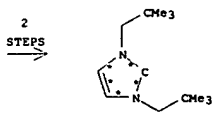
R



● Ag(I)

S

L62 ANSWER 1 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



U
YIELD 55%

RX(7) RCT Q 78198-90-0, R 18997-19-8, S 2923-28-6
PRO T 883990-73-6
SOL 75-09-2 CH2Cl2
CON 24 hours, 50 deg C
NTE in the dark

RX(8) RCT T 883990-73-6
RGT L 7693-26-7 KH
PRO U 881020-60-6
SOL 109-99-9 THF
CON overnight, -78 deg C -> room temperature

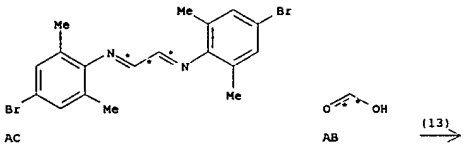
L62 ANSWER 2 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 144:171093 CASREACT
TITLE: π-face donor properties of N-heterocyclic carbenes
AUTHOR(S): Suessner, Marcus; Plenio, Herbert
CORPORATE SOURCE: Anorganische Chemie im Zintl-Institut des FB Chemie, TU Darmstadt, Darmstadt, 64287, Germany
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2005), (43), 5417-5419
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The donor properties of aryl-substituted N-heterocyclic carbenes (NHC) were characterized by lone pair donation from the carbene C and, as is shown here, by donation of electron d. of the aromatic π-face of the NHC aryl groups towards the metal. The variation of the remote substituents R (R = H, OC12H25, Me, Br) on the Ph ring of ruthenium diphenyl-substituted imidazolylidene-based NHC complexes has a significant influence on the redox behavior of these Grubbs II and Grubbs-Hoveyda type metathesis catalysts, and can be used to modify the catalytic activity of such complexes. As evidenced by cyclic voltammetric studies of Grubbs-Hoveyda type complexes, the saturated and unsatd. NHC ligands can give rise to different redox potentials Ru(II)/Ru(III). The systematic changes of the redox potential according to the electron-donating nature of the remote substituents and the fact that the aryl ring is electronically decoupled from the N heterocycles provides strong evidence of the π-face coordination of the Ru-carbene.

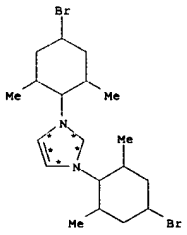
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(13) OF 102 ...AC + AB ===> I...



AC AB

L62 ANSWER 2 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

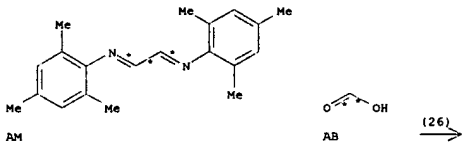


● Cl⁻

I

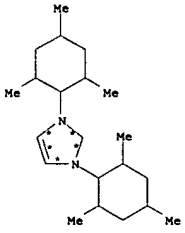
RX(13) RCT AC 181709-91-1, AB 64-18-6
RGT AD 7647-01-0 HCl
PRO I 221154-71-8
SOL 123-91-1 Dioxane
NTE conditions not stated

RX(26) OF 102 ...AM + AB ===> A...



AM AB

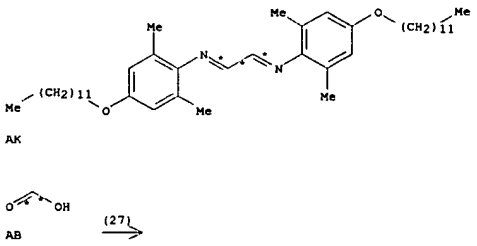
L62 ANSWER 2 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



A

RX(26) RCT AM 56222-36-7, AB 64-18-6
RGT AD 7647-01-0 HCl
PRO A 160256-31-5
SOL 123-91-1 Dioxane
NTE conditions not stated

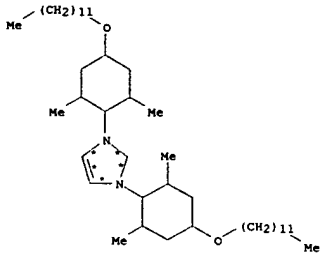
RX(27) OF 102 ...AK + AB ===> AV...



AK

AB

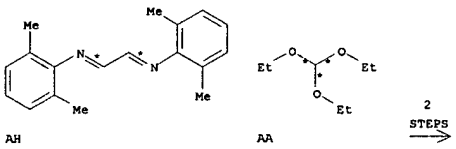
L62 ANSWER 2 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



AV

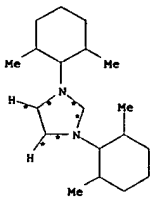
RX(27) RCT AK **874184-80-2**, AB 64-18-6
RGT AD 7647-01-0 HCl
PRO AV **874184-82-4**
SOL 123-91-1 Dioxane
NTE conditions not stated

RX(42) OF 102 COMPOSED OF RX(16), RX(29)
RX(42) **AH** + AA ===> **AW**



AH AA

L62 ANSWER 2 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

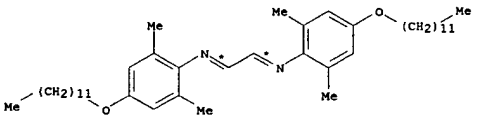


AW

RX(16) RCT AH **49673-43-0**
RGT AJ 16853-85-3 LiAlH4
PRO AI 475578-15-5
SOL 109-99-9 THF
NTE conditions not stated

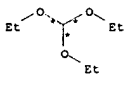
RX(29) RCT AI 475578-15-5, AA 122-51-0
RGT AB 64-18-6 HCO2H
PRO AW **741245-49-8**
NTE solvent and conditions not stated

RX(43) OF 102 COMPOSED OF RX(17), RX(30)
RX(43) **AK** + AA ===> **AX**

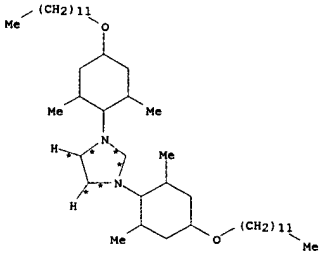


AK

L62 ANSWER 2 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



AA



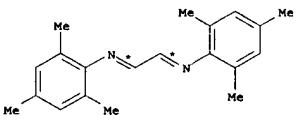
AX

RX(17) RCT AK **874184-80-2**
RGT AJ 16853-85-3 LiAlH4
PRO AL 874184-78-8
SOL 109-99-9 THF
NTE conditions not stated

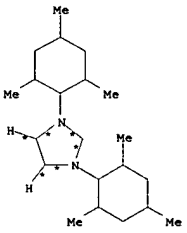
RX(30) RCT AL 874184-78-8, AA 122-51-0
RGT AB 64-18-6 HCO2H
PRO AX **874184-84-6**
NTE solvent and conditions not stated

RX(44) OF 102 COMPOSED OF RX(18), RX(31)
RX(44) **AM** + AA ===> **G**

L62 ANSWER 2 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



AM AA



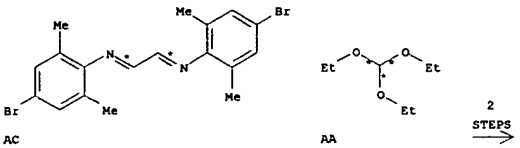
G

RX(18) RCT AM **56222-36-7**
RGT AJ 16853-85-3 LiAlH4
PRO AN 258278-23-8
SOL 109-99-9 THF
NTE conditions not stated

RX(31) RCT AN 258278-23-8, AA 122-51-0
RGT AB 64-18-6 HCO2H
PRO G **245679-17-8**
NTE solvent and conditions not stated

RX(45) OF 102 COMPOSED OF RX(19), RX(12)
RX(45) **AC** + AA ===> **K**

L62 ANSWER 2 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



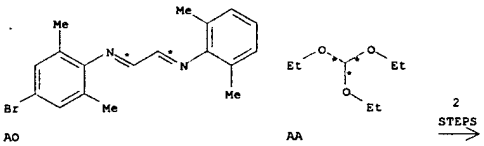
AC AA 2 STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(19) RCT AC 101709-91-1
RGT AJ 16853-85-3 LiAlH4
PRO Z 870123-16-3
SOL 109-99-9 THF
NTE conditions not stated

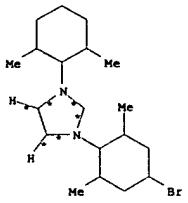
RX(12) RCT Z 870123-16-3, AA 122-51-0
RGT AB 64-18-6 HCO2H
PRO K 874184-69-7
NTE solvent and conditions not stated

RX(46) OF 102 COMPOSED OF RX(20), RX(32)
RX(46) AO + AA ===> AF



AO AA 2 STEPS

L62 ANSWER 2 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



AF

RX(20) RCT AO 874184-81-3
RGT AJ 16853-85-3 LiAlH4
PRO AP 874184-79-9
SOL 109-99-9 THF
NTE conditions not stated

RX(32) RCT AP 874184-79-9, AA 122-51-0
RGT AB 64-18-6 HCO2H
PRO AF 874184-85-7
NTE solvent and conditions not stated

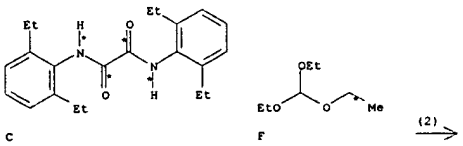
L62 ANSWER 3 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:439653 CASREACT
TITLE: Room-Temperature Negishi Cross-Coupling of Unactivated Alkyl Bromides with Alkyl Organozinc Reagents Utilizing a Pd/N-Heterocyclic Carbene Catalyst
AUTHOR(S): Hadei, Niloufar; Kantchev, Eric Assen B.; O'Brien, Christopher J.; Organ, Michael G.
CORPORATE SOURCE: Department of Chemistry, York University, Toronto, ON, M3J 1P3, Can.
SOURCE: Journal of Organic Chemistry (2005), 70(21), 8503-8507
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A high-yielding cross-coupling reaction of unactivated alkyl bromides possessing β-hydrogens with alkylzinc halides utilizing a Pd/N-heterocyclic carbene (NHC) catalyst at room temperature is described. A variety of Pd sources, Pd2(dba)3, Pd(OAc)2, or PdBr2, with the com. available ligand precursor 1,3-bis(2,6-diisopropylphenyl)imidazolium chloride successfully coupled 1-bromo-3-phenylpropane with n-butylzinc bromide in THF/NMP. An investigation of different NHC precursors showed that the bulky 2,6-diisopropylphenyl moiety was necessary to achieve high coupling yields (75-85%). The corresponding Et analog was moderately active (11%). A range of unsym. NHC precursors were prepared and evaluated. The ligand precursor containing one 2,6-diisopropylphenyl and one 2,6-diethylphenyl afforded the coupling product in 47% yield, clearly suggesting a direct relationship between the steric topog. created by the flanking N-substituents and catalyst activity. Under optimal conditions, a number of alkyl bromides and alkylzinc halides possessing common functional groups (amide, nitrile, ester, acetal, and alkyne) were effectively coupled (61-92%). It is noteworthy that β-substituted alkyl bromides and alkylzinc halides successfully underwent cross-coupling. Also, under these conditions alkyl chlorides were unaffected.

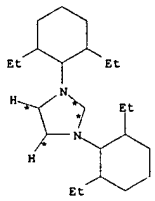
REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 34 ...C + F ===> G



C F (2)

L62 ANSWER 3 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Cl⁻

G
YIELD 56%

RX(2) RCT C 118923-23-2

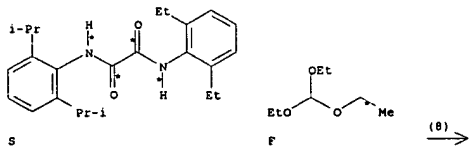
STAGE(1)
RGT H 14044-65-6 BH3-THF
SOL 109-99-9 THF
CON 18 hours, reflux

STAGE(2)
RGT I 67-56-1 MeOH
CON room temperature

STAGE(3)
RCT F 122-51-0
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water, 122-51-0 CH(OEt)3
CON 2 hours, 120 deg C

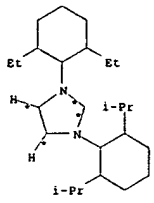
PRO G 868593-18-4

RX(8) OF 34 ...S + F ===> AA



S F (8)

L62 ANSWER 3 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Cl⁻

AA
YIELD 78%

RX(8) RCT S 868593-23-1

STAGE(1)
RGT H 14044-65-6 BH3-THF
SOL 109-99-9 THF
CON 18 hours, reflux

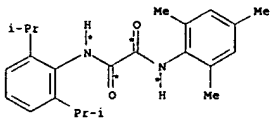
STAGE(2)
RGT I 67-56-1 MeOH
CON room temperature

STAGE(3)
RCT F 122-51-0
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water, 122-51-0 CH(OEt)3
CON 2 hours, 120 deg C

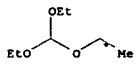
PRO AA 866926-58-1

RX(9) OF 34 ...V + F ===> AB

L62 ANSWER 3 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

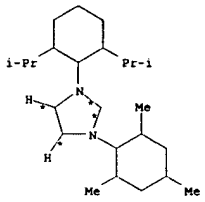


V



F

(9)



● Cl⁻

AB
YIELD 52%

RX(9) RCT V 868593-25-3

STAGE(1)
RGT H 14044-65-6 BH3-THF
SOL 109-99-9 THF
CON 18 hours, reflux

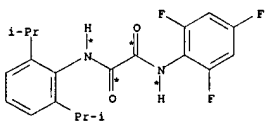
STAGE(2)
RGT I 67-56-1 MeOH
CON room temperature

STAGE(3)
RCT F 122-51-0
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water, 122-51-0 CH(OEt)3
CON 2 hours, 120 deg C

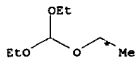
L62 ANSWER 3 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO AB 866926-59-2

RX(10) OF 34 ...X + F ===> AC

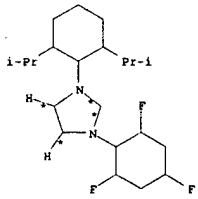


X



F

(10)



● Cl⁻

AC
YIELD 82%

RX(10) RCT X 868593-27-5

STAGE(1)
RGT H 14044-65-6 BH3-THF
SOL 109-99-9 THF
CON 24 hours, reflux

STAGE(2)
RGT I 67-56-1 MeOH
CON room temperature

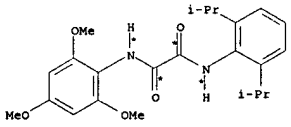
STAGE(3)
RCT F 122-51-0
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water, 122-51-0 CH(OEt)3

L62 ANSWER 3 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

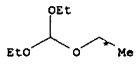
CON 2 hours, 120 deg C

PRO AC 868593-33-3

RX(11) OF 34 ...Z + F ===> AD

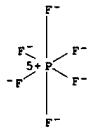


Z

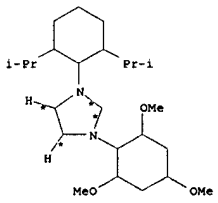


F

(11)



AD: CM 1
YIELD 37%



AD: CM 2
YIELD 37%

RX(11) RCT Z 868593-29-7

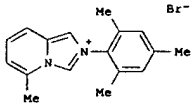
STAGE(1)
RGT H 14044-65-6 BH3-THF
SOL 109-99-9 THF
CON 24 hours, reflux

STAGE(2)
RGT I 67-56-1 MeOH
CON room temperature

STAGE(3)
RCT F 122-51-0
RGT AE 16941-11-0 PF6.NH4
SOL 109-99-9 THF
CON 18 hours, 80 deg C

L62 ANSWER 3 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
PRO AD 868593-36-6

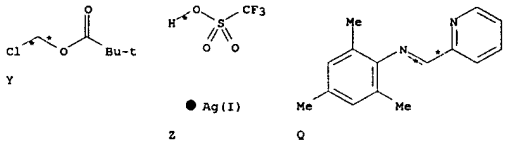
L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 143:172810 CASREACT
TITLE: Imidazo[1,5-a]pyridine-3-ylidenes-pyridine derived N-heterocyclic carbene ligands
AUTHOR(S): Burstein, Christian; Lehmann, Christian W.; Glorius, Frank
CORPORATE SOURCE: Max-Planck-Institut fuer Kohlenforschung, Muelheim an der Ruhr, 45470, Germany
SOURCE: Tetrahedron (2005), 61(26), 6207-6217
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

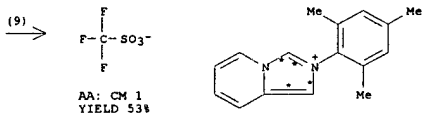
AB The ready synthesis of differently substituted 2H-imidazo[1,5-a]pyridin-4-ium bromides, e.g., I, is reported. These salts were precursors for a class of N-heterocyclic carbene ligands. As a consequence of their bicyclic geometry, these ligands are capable of influencing the coordination sphere of a carbene bound metal. The usefulness of these ligands was demonstrated in the palladium-catalyzed Suzuki-Miyaura cross-coupling of sterically hindered aryl chlorides.
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(9) OF 53 ...Y + Z + Q ===> AA



Y Z Q

L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



AA: CM 1
YIELD 53%

AA: CM 2
YIELD 53%

RX(9) RCT Y 18997-19-8, Z 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

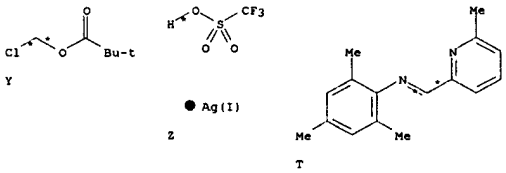
STAGE(2)
RCT Q 861404-00-4
CON SUBSTAGE(1) 19 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

STAGE(3)
SOL 67-56-1 MeOH

STAGE(4)
RGT AB 1643-19-2 Bu4N.Br
SOL 75-09-2 CH2Cl2
CON 2 hours, room temperature

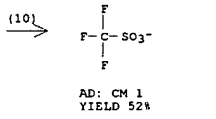
PRO AA 861404-15-1
NTE in the dark

RX(10) OF 53 ...Y + Z + T ===> AD

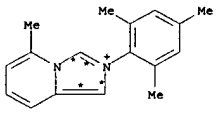


Y Z T

L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



AD: CM 1
YIELD 52%



AD: CM 2
YIELD 52%

RX(10) RCT Y 18997-19-8, Z 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT T 861404-01-5
CON SUBSTAGE(1) 24 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

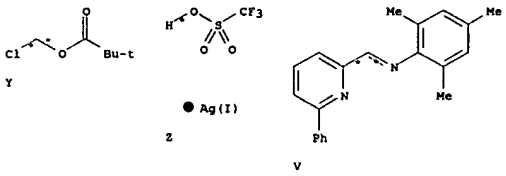
STAGE(3)
SOL 64-17-5 EtOH

STAGE(4)
RGT AB 1643-19-2 Bu4N.Br
SOL 75-09-2 CH2Cl2
CON 2 hours, room temperature

PRO AD 861404-16-2
NTE in the dark

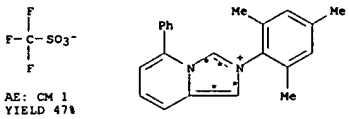
RX(11) OF 53 ...Y + Z + V ===> AE

L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



Y Z V

(11)



AE: CM 1
YIELD 47%

AE: CM 2
YIELD 47%

RX(11) RCT Y 18997-19-8, Z 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT V 861404-02-6
CON SUBSTAGE(1) 14 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

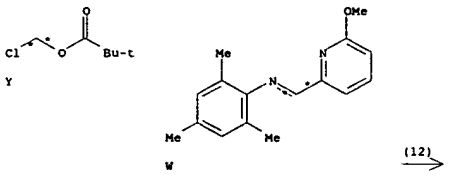
STAGE(3)
SOL 64-17-5 EtOH

STAGE(4)
RGT AB 1643-19-2 Bu4N.Br
SOL 75-09-2 CH2Cl2
CON 12 hours, room temperature

PRO AE 861404-18-4

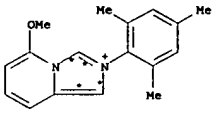
L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
NTE in the dark

RX(12) OF 53 ...Y + W ===> AF



Y W

(12)



AF
YIELD 22%

RX(12) RCT Y 18997-19-8

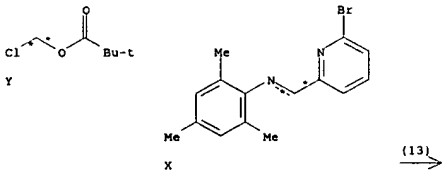
STAGE(1)
RGT Z 2923-28-6 AgO3SCF3
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT W 861404-03-7
CON SUBSTAGE(1) 20 hours, 45 deg C
SUBSTAGE(2) 45 deg C -> room temperature

STAGE(3)
SOL 64-17-5 EtOH
CON room temperature

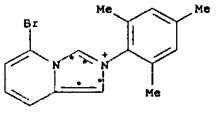
L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
PRO AF 861404-08-2
NTE in the dark

RX(13) OF 53 ...Y + X ===> AG...



Y X

(13)



AG
YIELD 54%

RX(13) RCT Y 18997-19-8

STAGE(1)
RGT Z 2923-28-6 AgO3SCF3
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

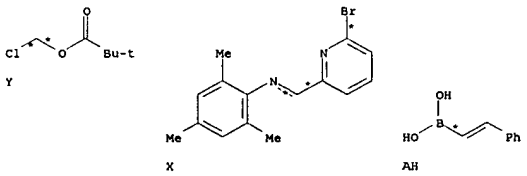
STAGE(2)
RCT X 861404-04-8
CON SUBSTAGE(1) 17 hours, 45 deg C
SUBSTAGE(2) 45 deg C -> room temperature

STAGE(3)
SOL 64-17-5 EtOH
CON room temperature

PRO AG 861404-09-3
NTE in the dark

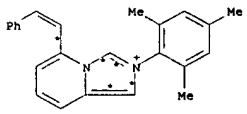
L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(33) OF 53 COMPOSED OF RX(13), RX(14)
RX(33) Y + X + AH ===> AI



Y X AH

2
STEPS



AI
YIELD 97%

RX(13) RCT Y 18997-19-8

STAGE(1)
RGT Z 2923-28-6 AgO3SCF3
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT X 861404-04-8
CON SUBSTAGE(1) 17 hours, 45 deg C
SUBSTAGE(2) 45 deg C -> room temperature

STAGE(3)
SOL 64-17-5 EtOH
CON room temperature

L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO AG 861404-09-3
NTE in the dark

RX(14) RCT AG 861404-09-3

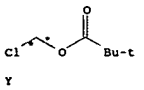
STAGE(1)
CAT 14221-01-3 Pd(PPh3)4
SOL 110-71-4 (CH2OMe)2
CON 30 minutes, room temperature

STAGE(2)
RCT AH 4363-35-3
RGT AJ 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON 25 hours

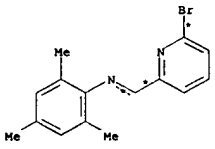
STAGE(3)
SOL 7732-18-5 Water
CON room temperature

PRO AI 861404-11-7

RX(34) OF 53 COMPOSED OF RX(13), RX(15)
RX(34) Y + X + AM ===> AN

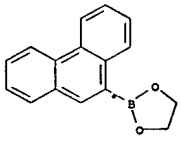


Y



X

L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



AM

2 STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(13) RCT Y 18997-19-8

STAGE(1)
RGT Z 2923-28-6 AgO3SCF3
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT X 861404-04-8
CON SUBSTAGE(1) 17 hours, 45 deg C
SUBSTAGE(2) 45 deg C -> room temperature

STAGE(3)
SOL 64-17-5 EtOH
CON room temperature

PRO AG 861404-09-3
NTE in the dark

RX(15) RCT AG 861404-09-3

STAGE(1)
CAT 14221-01-3 Pd(PPh3)4
SOL 110-71-4 (CH2OMe)2
CON 30 minutes, room temperature

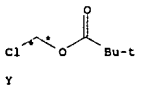
STAGE(2)
RCT AM 861404-10-6
RGT AJ 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON SUBSTAGE(1) 4 hours, 80 deg C
SUBSTAGE(2) 80 deg C -> room temperature

STAGE(3)
SOL 7732-18-5 Water
CON room temperature

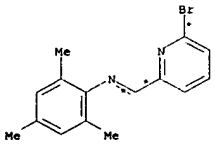
L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO AN 861404-12-8

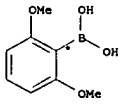
RX(35) OF 53 COMPOSED OF RX(13), RX(16)
RX(35) Y + X + AO ===> AP



Y

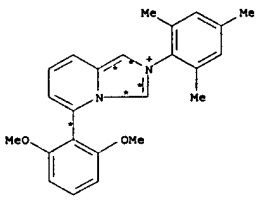


X



AO

2 STEPS



● Br⁻

AP
YIELD 68%

RX(13) RCT Y 18997-19-8

STAGE(1)
RGT Z 2923-28-6 AgO3SCF3
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)

L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RCT X 861404-04-8
CON SUBSTAGE(1) 17 hours, 45 deg C
SUBSTAGE(2) 45 deg C -> room temperature

STAGE(3)
SOL 64-17-5 EtOH
CON room temperature

PRO AG 861404-09-3
NTE in the dark

RX(16) RCT AG 861404-09-3

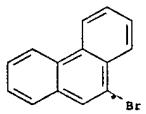
STAGE(1)
CAT 14221-01-3 Pd(PPh3)4
SOL 110-71-4 (CH2OMe)2
CON 30 minutes, room temperature

STAGE(2)
RCT AO 23112-96-1
RGT AJ 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON SUBSTAGE(1) 18 hours, 80 deg C
SUBSTAGE(2) 6 hours, 80 deg C
SUBSTAGE(3) 80 deg C -> room temperature

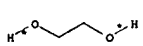
STAGE(3)
SOL 7732-18-5 Water
CON room temperature

PRO AP 861404-13-9

RX(49) OF 53 COMPOSED OF REACTION SEQUENCE RX(17), RX(15)
AND REACTION SEQUENCE RX(13), RX(15)
...AQ + AR ===> AM...
...Y + X + AM ===> AN



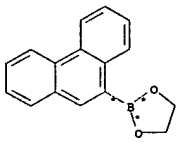
AQ



AR

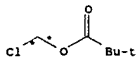
2 STEPS

L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

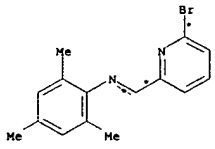


AM

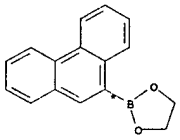
START NEXT REACTION SEQUENCE



Y



X



AM

2 STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(17) RCT AQ 573-17-1

STAGE(1)
RGT AS 7553-56-2 I2, AT 75-03-6 EtI, AU 7439-95-4 Mg
SOL 109-99-9 THF
CON 1 hour, room temperature

L62 ANSWER 4 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(2)
RGT AV 121-43-7 Me borate
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> room temperature

STAGE(3)
RCT AR 107-21-1
SOL 108-88-3 PhMe
CON overnight, reflux

PRO AM 861404-10-6

RX(13) RCT Y 18997-19-8

STAGE(1)
RGT Z 2923-28-6 AgO3SCF3
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT X 861404-04-8
CON SUBSTAGE(1) 17 hours, 45 deg C
SUBSTAGE(2) 45 deg C -> room temperature

STAGE(3)
SOL 64-17-5 EtOH
CON room temperature

PRO AG 861404-09-3
NTE in the dark

RX(15) RCT AG 861404-09-3

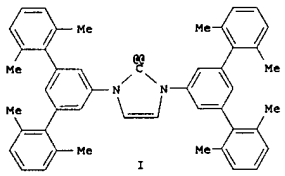
STAGE(1)
CAT 14221-01-3 Pd(PPh3)4
SOL 110-71-4 (CH2OMe)2
CON 30 minutes, room temperature

STAGE(2)
RCT AM 861404-10-6
RGT AJ 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON SUBSTAGE(1) 4 hours, 80 deg C
SUBSTAGE(2) 80 deg C -> room temperature

STAGE(3)
SOL 7732-18-5 Water
CON room temperature

PRO AN 861404-12-8

L62 ANSWER 5 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 143:60075 CASREACT
TITLE: Fixation of Both O2 and CO2 from Air by a Crystalline Palladium Complex Bearing N-Heterocyclic Carbene Ligands
AUTHOR(S): Yamashita, Makoto; Goto, Kei; Kawashima, Takayuki
CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, University of Tokyo, Bunkyo, Tokyo, 113-0033, Japan
SOURCE: Journal of the American Chemical Society (2005), 127(20), 7294-7295
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Crystals of the two-coordinate Pd(0) complex Pd(ITmt)2 (1) bearing the new N-heterocyclic carbene ligand I (ITmt), directly and rapidly fixed both O2 and CO2 from air to produce the corresponding Pd(II) peroxocarbonate complex [Pd(ITmt)2O2CO2] (2). The present reaction consists of dioxygenation of the Pd(0) complex 1 to the Pd(II) peroxo complex [Pd(ITmt)2O2] (3) and the subsequent CO2 insertion to produce the peroxocarbonate complex 2. Reaction of the crystals of 1 with air was monitored by microscopic IR spectroscopy to confirm the sequence of the two-step solid-state reaction. The unique reactivity of solid 1 toward air was explained in terms of the structural features of the carbene ligand, ITmt.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(4) OF 36 ...Q + N ===> R...

L62 ANSWER 5 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

Q

N

(4)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4) RCT Q 50-00-0

STAGE(1)
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 120 deg C
SUBSTAGE(2) 120 deg C -> room temperature

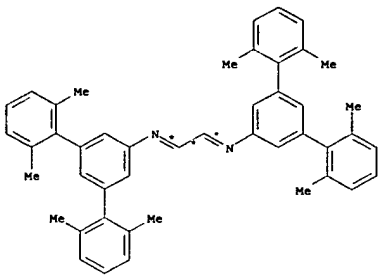
STAGE(2)
RCT N 854030-35-6
RGT S 7647-01-0 HCl
SOL 60-29-7 Et2O, 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, 120 deg C
SUBSTAGE(2) 120 deg C -> room temperature

PRO R 854030-33-4
NTE paraformaldehyde used

RX(13) OF 36 COMPOSED OF RX(4), RX(5)
RX(13) Q + N ===> U

Q

L62 ANSWER 5 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



N

2 STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4) RCT Q 50-00-0

STAGE(1)
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 120 deg C
SUBSTAGE(2) 120 deg C -> room temperature

STAGE(2)
RCT N **854030-35-6**
RGT S 7647-01-0 HCl
SOL 60-29-7 Et2O, 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, 120 deg C
SUBSTAGE(2) 120 deg C -> room temperature

PRO R 854030-33-4
NTE paraformaldehyde used

RX(5) RCT R 854030-33-4
RGT V 865-47-4 t-BuOK
PRO U **854030-37-8**
SOL 60-29-7 Et2O, 109-99-9 THF
CON 1.5 hours, room temperature

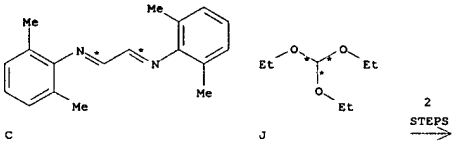
L62 ANSWER 6 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:354850 CASREACT
TITLE: Regarding the Mechanism of Olefin Metathesis with Sol-Gel-Supported Ru-Based Complexes Bearing a Bidentate Carbene Ligand. Spectroscopic Evidence for Return of the Propagating Ru Carbene
AUTHOR(S): Kingsbury, Jason S.; Hoveyda, Amir H.
CORPORATE SOURCE: Department of Chemistry, Merkert Chemistry Center, Boston College, Chestnut Hill, MA, 02467, USA
SOURCE: Journal of the American Chemical Society (2005), 127(12), 4510-4517
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two isotopically and structurally labeled Ru-based carbenes have been prepared and attached to the surface of monolithic sol-gel glass. The resulting glass-supported complexes exhibit significant catalytic activity in promoting olefin metathesis reactions and provide products of high purity. Through anal. of the derivatized glass pellets used in a sequence of catalytic ring-closing metathesis reactions mediated by various supported Ru carbenes, it is demonstrated that free Ru carbene intermediates in solution can be scavenged by support-bound styrene ether ligands prior to the onset of competing transition metal decomposition The observations detailed herein provide rigorous evidence that the initially proposed release/return mechanism is, at least partially, operative. The present investigations shed light on a critical aspect of the mechanism of an important class of Ru-based metathesis complexes (those bearing a bidentate styrene ether ligand).

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(16) OF 39 COMPOSED OF RX(2), RX(3)
RX(16) C + J ===> K

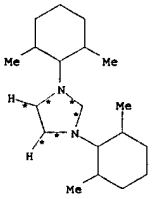


C J

2 STEPS

L62 ANSWER 6 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

K: CM 1
YIELD 90%



K: CM 2
YIELD 90%

RX(2) RCT C **49673-43-0**

STAGE(1)
RGT G 25895-60-7 NaBH3CN
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 10 minutes, 0 deg C

STAGE(2)
RGT H 7647-01-0 HCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) 0 deg C, acidify
SUBSTAGE(2) 0 deg C -> 22 deg C
SUBSTAGE(3) 30 minutes, 22 deg C

STAGE(3)
RGT I 1310-58-3 KOH
SOL 7732-18-5 Water
CON room temperature, pH 8 - 9

PRO F 72991-60-7
NTE acidification in stage 2 repeated 3 times total

RX(3) RCT F 72991-60-7, J 122-51-0
RGT L 13826-83-0 NH4.BF4
PRO K **848979-23-7**
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 10 hours, 120 deg C

L62 ANSWER 6 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
SUBSTAGE(3) 120 deg C -> 22 deg C

L62 ANSWER 7 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:347439 CASREACT

TITLE: Synthesis, spectroscopic and electrochemical properties of some heteroleptic tris-chelates of ruthenium(II) involving 2,2'-bipyridine (bpy) and N-(aryl)pyridine-2-aldimine (L): X-ray crystal structures of [Ru(bpy)(L2)2](ClO4)2·H2O and 3-N-(4-tolyl)imidazo[1,5a]pyridinium perchlorate

AUTHOR(S): Mishra, Dipankar; Naskar, Subhendu; Adhikary, Bibhutosh; Butcher, Raymond J.; Chattopadhyay, Shyamal Kumar

CORPORATE SOURCE: Department of Chemistry, Bengal Engineering and Science University, Howrah, Shibpur, 711 103, India

SOURCE: Polyhedron (2005), 24(2), 201-208
CODEN: PLYHDE; ISSN: 0277-5387

PUBLISHER: Elsevier B.V.

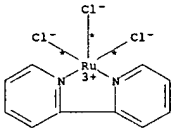
DOCUMENT TYPE: Journal

LANGUAGE: English

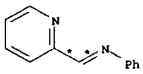
AB Four ruthenium (II) complexes [Ru(bpy)(L1)2](ClO4)2·H2O (A1), [Ru(bpy)(L2)2](ClO4)2·H2O (A2), [Ru(bpy)(L3)2](ClO4)2·H2O (A3), [Ru(bpy)(L4)2](ClO4)2·H2O (A4) (L1 = phenyl(2-pyridylmethylene)amine, L2 = (4-methylphenyl)(2-pyridylmethylene)amine, L3 = (4-chlorophenyl)(2-pyridylmethylene)amine, L4 = (4-fluorophenyl)(2-pyridylmethylene)amine and bpy = 2,2'-bipyridyl) were synthesized. In addition to these ruthenium complexes, the authors also were able to isolate four imidazopyridinium perchlorate compds. B1-B4 from the same reactions. The x-ray crystal structures of one representative ruthenium complex (A2) and the imidazopyridinium perchlorate compound (B2) were determined The Ru(II) center in the complex is coordinated by six N donors with a distorted octahedral geometry. The imine ligands (L) act as bidentate N,N donors.

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

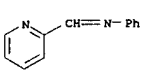
RX(1) OF 4 A + 3 B + C ===> D + E



A

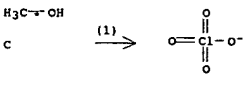


B



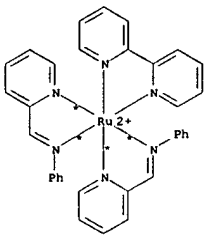
2 B

L62 ANSWER 7 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



C

D: CM 1



D: CM 2

E: CM 1

E: CM 2

RX(1) RCT A 69141-04-4, B 7032-25-9, C 67-56-1

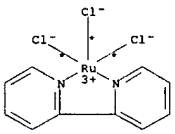
STAGE(1)
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) 4 hours, reflux
SUBSTAGE(3) reflux -> room temperature

STAGE(2)
RGT F 7601-89-0 NaClO4
SOL 67-56-1 MeOH
CON room temperature

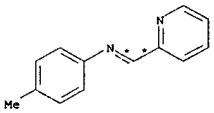
PRO D 848303-98-0, E 848304-04-1
NTE safety - product is a potentially explosive perchlorate salt

RX(2) OF 4 A + 3 G + C ===> H + I

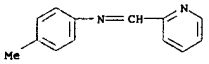
L62 ANSWER 7 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



A



G



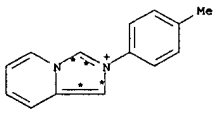
2 G

C

H: CM 1
YIELD 31%

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

I: CM 1
YIELD 36%



I: CM 2
YIELD 36%

RX(2) RCT A 69141-04-4, G 7471-13-8, C 67-56-1

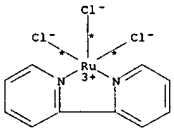
STAGE(1)
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) 4 hours, reflux
SUBSTAGE(3) reflux -> room temperature

STAGE(2)
RGT F 7601-89-0 NaClO4
SOL 67-56-1 MeOH
CON room temperature

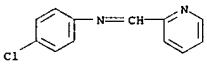
PRO H 156843-38-8, I 738585-87-0
NTE safety - product is a potentially explosive perchlorate salt

L62 ANSWER 7 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

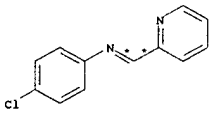
RX(3) OF 4 A + 3 J + C ===> K + L



A



2 J



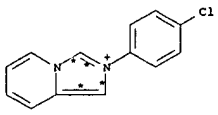
J

C

K: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L: CM 1



L: CM 2

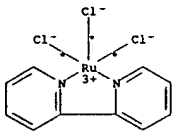
RX(3) RCT A 69141-04-4, J 26825-34-3, C 67-56-1

STAGE(1)
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) 4 hours, reflux
SUBSTAGE(3) reflux -> room temperature

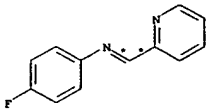
STAGE(2)
RGT F 7601-89-0 NaClO4
SOL 67-56-1 MeOH
CON room temperature

L62 ANSWER 7 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
PRO K 848304-00-7, L 738585-89-2
NTE safety - product is a potentially explosive perchlorate salt

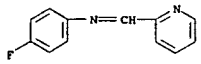
RX(4) OF 4 A + 3 M + C ===> N + O



A



M



2 M

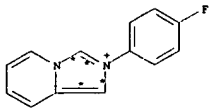
C

(4)

N: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

O: CM 1



O: CM 2

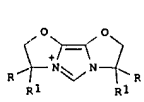
RX(4) RCT A 69141-04-4, M 29202-06-0, C 67-56-1

STAGE(1)
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) 4 hours, reflux
SUBSTAGE(3) reflux -> room temperature

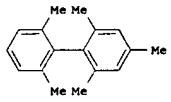
L62 ANSWER 7 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
STAGE(2)
RGT F 7601-89-0 NaClO4
SOL 67-56-1 MeOH
CON room temperature

PRO N 848304-02-9, O 848304-06-3
NTE safety - product is a potentially explosive perchlorate salt

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 142:93738 CASREACT
TITLE: Sterically demanding, bioxazoline-derived N-heterocyclic carbene ligands with restricted flexibility for catalysis
AUTHOR(S): Altenhoff, Gereon; Goddard, Richard; Lehmann, Christian W.; Glorius, Frank
CORPORATE SOURCE: Max-Planck-Institut fuer Kohlenforschung, Muelheim an der Ruhr, 45470, Germany
SOURCE: Journal of the American Chemical Society (2004), 126(46), 15195-15201
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

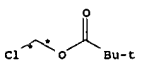


II

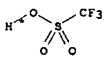
AB The triflate salts of imidazobioxazolium ions I [R = R1 = Me; RR1 = (CH2)n; n = 5, 6, 7, 8, 12] are prepared as precursors for sterically demanding and conformationally constrained N-heterocyclic carbene (NHC) ligands; palladium complexes derived from I [RR1 = (CH2)n; n = 7, 12] act as effective catalysts for the Suzuki-Miyaura coupling reactions of ortho-substituted aryl chlorides with ortho-substituted arylboronic acids to provide triortho- and tetraortho-substituted biaryls such as II in 47-96% yields. I•CF3SO3- are prepared in five steps from α,α-disubstituted amino acids and di-Et oxalate; reduction of amino acids to the amino alcs., condensation of the amino alcs. with di-Et oxalate to give the hydroxymethyl-substituted oxamides, chlorination of the primary alc. moieties, cyclization of the oxamide with the chloromethyl groups to give the bioxazolines, and reaction of the bioxazolines with chloromethyl pivalate and silver triflate. I•CF3SO3- are soluble in methylene chloride and THF and are chromatographable. Iridium cyclooctadienyl and iridium dicarbonyl chloride complexes derived from I•CF3SO3- [R = R1 = Me; RR1 = (CH2)n; n = 6, 8 , 12] are prepared; IR frequencies of the carbonyl ligands indicate that carbene ligands derived from I•CF3SO3- are less electron-donating than previous NHC ligands but are comparable to electron-rich phosphines. Selected iridium cyclooctadienyl and iridium dicarbonyl chloride complexes of imidazobioxazolium ligands are characterized by X-ray crystallog. Dimeric palladium chloride complexes derived from I•CF3SO3- [RR1 = (CH2)n; n = 7 , 12] are prepared and characterized by X-ray crystallog. Generation of the carbene ligand from I•CF3SO3- [RR1 = (CH2)12] by treatment with potassium hydride and potassium tert-butoxide followed by addition of palladium acetate yields a palladium catalyst which is effective for the Suzuki-Miyaura coupling of highly hindered aryl chlorides and arylboronic acids. Potassium phosphate is the most effective base and toluene is the most effective solvent for Suzuki-Miyaura coupling of highly hindered aryl chlorides and arylboronic acids using imidazobioxazolium-derived carbene ligands, although cesium carbonate can also be used as the base and 1,4-dioxane as the solvent; the isolated dimeric palladium chloride complexes derived from I•CF3SO3- [RR1 = (CH2)n; n = 7, 12] can also be used as catalysts. Anhyd. conditions are important to minimize hydrodeborylation byproducts of the coupling reaction. E.g., in the presence of the palladium catalyst generated from I•CF3SO3- [RR1 = (CH2)12] and palladium acetate and potassium phosphate, 2-chloro-1,3-dimethylbenzene and 2,4,6-trimethylphenylboronic acid undergo coupling in toluene at 100° for 16 h to provide biphenyl II in 96% yield.

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

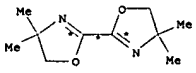
RX(23) OF 154 ...AP + AQ + AI ===> AR...



AP



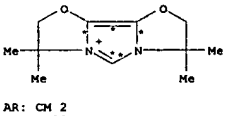
AQ



AI

(23)

AR: CM 1
YIELD 83%



AR: CM 2
YIELD 83%

RX(23) RCT AP 18997-19-8, AQ 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

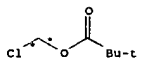
STAGE(2)
RCT AI 49585-66-2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

STAGE(3)

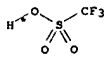
L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
RGT E 67-56-1 MeOH

PRO AR **814254-77-8**
NTE sealed tube (2nd stage), in the dark (2nd stage)

RX(24) OF 154 ...AP + AQ + **AK** ===> **AT**

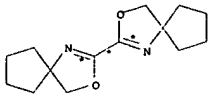


AP



● Ag(I)

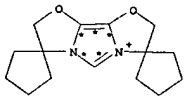
AQ



AK

(24)

AT: CM 1
YIELD 65%



AT: CM 2
YIELD 65%

RX(24) RCT AP 18997-19-8, AQ 2923-28-6

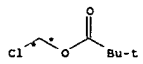
STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT AK **814254-72-3**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

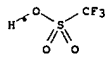
L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
STAGE(3)
RGT E 67-56-1 MeOH

PRO AT **814254-79-0**
NTE sealed tube (2nd stage), in the dark (2nd stage)

RX(25) OF 154 ...AP + AQ + **AL** ===> **AU**...

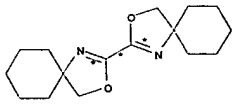


AP



● Ag(I)

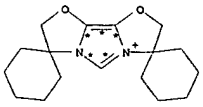
AQ



AL

(25)

AU: CM 1
YIELD 85%



AU: CM 2
YIELD 85%

RX(25) RCT AP 18997-19-8, AQ 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

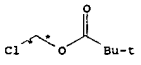
STAGE(2)
RCT AL **606970-67-6**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

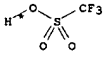
STAGE(3)
RGT E 67-56-1 MeOH

PRO AU **606970-69-8**
NTE sealed tube (2nd stage), in the dark (2nd stage)

RX(26) OF 154 ...AP + AQ + **AM** ===> **AV**...

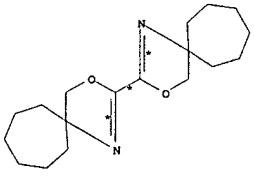


AP



● Ag(I)

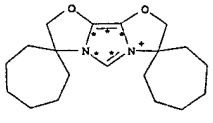
AQ



AM

(26)

AV: CM 1
YIELD 63%



AV: CM 2
YIELD 63%

RX(26) RCT AP 18997-19-8, AQ 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

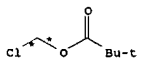
STAGE(2)
RCT AM **814254-73-4**

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

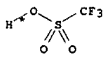
STAGE(3)
RGT E 67-56-1 MeOH

PRO AV **814254-81-4**
NTE sealed tube (2nd stage), in the dark (2nd stage)

RX(27) OF 154 ...AP + AQ + **AN** ===> **AW**...

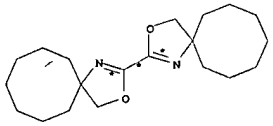


AP



● Ag(I)

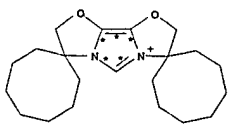
AQ



AN

(27)

AW: CM 1
YIELD 61%



AW: CM 2
YIELD 61%

RX(27) RCT AP 18997-19-8, AQ 2923-28-6

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

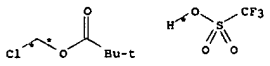
STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT AN **814254-74-5**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

STAGE(3)
RGT E 67-56-1 MeOH

PRO AW **814254-83-6**
NTE sealed tube (2nd stage), in the dark (2nd stage)

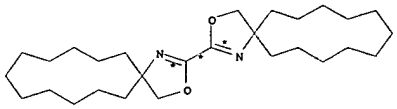
RX(28) OF 154 ...AP + AQ + **AO** ===> **AX**...



AP

● Ag(I)

AQ

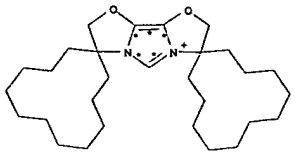


AO

(28)

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

AX: CM 1
YIELD 60%



AX: CM 2
YIELD 60%

RX(28) RCT AP 18997-19-8, AQ 2923-28-6

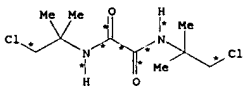
STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT AO **814254-75-6**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

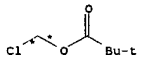
STAGE(3)
RGT E 67-56-1 MeOH

PRO AX **814254-85-8**
NTE sealed tube (2nd stage), in the dark (2nd stage)

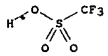
RX(69) OF 154 COMPOSED OF RX(17), RX(23)
RX(69) **AA** + AP + AQ ===> **AR**



AA



AP



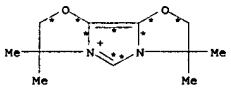
● Ag(I)

AQ

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

2 STEPS

AR: CM 1
YIELD 83%



AR: CM 2
YIELD 83%

RX(17) RCT AA **61051-14-7**
RGT F 1310-73-2 NaOH
PRO AI 49585-66-2
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(23) RCT AP 18997-19-8, AQ 2923-28-6

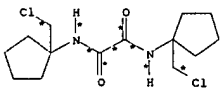
STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT AI 49585-66-2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

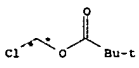
STAGE(3)
RGT E 67-56-1 MeOH

PRO AR **814254-77-8**
NTE sealed tube (2nd stage), in the dark (2nd stage)

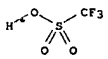
RX(70) OF 154 COMPOSED OF RX(18), RX(24)
RX(70) **AD** + AP + AQ ===> **AT**



AD



AP



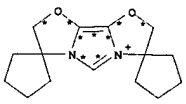
● Ag(I)

AQ

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

2 STEPS

AT: CM 1
YIELD 65%



AT: CM 2
YIELD 65%

RX(18) RCT AD **814254-68-7**
RGT F 1310-73-2 NaOH
PRO AK 814254-72-3
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(24) RCT AP 18997-19-8, AQ 2923-28-6

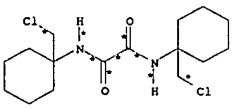
STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT AK 814254-72-3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

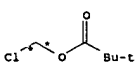
STAGE(3)
RGT E 67-56-1 MeOH

PRO AT **814254-79-0**
NTE sealed tube (2nd stage), in the dark (2nd stage)

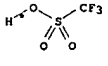
RX(71) OF 154 COMPOSED OF RX(19), RX(25)
RX(71) **AE** + AP + AQ ===> **AU**



AE



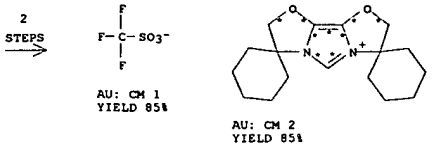
AP



● Ag(I)

AQ

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(19) RCT AE **606970-66-5**
RGT F 1310-73-2 NaOH
PRO AL 606970-67-6
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(25) RCT AP 18997-19-8, AQ 2923-28-6

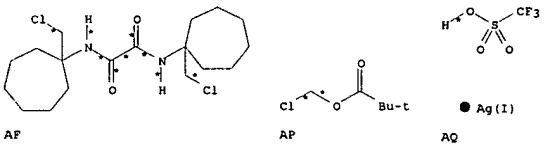
STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT AL 606970-67-6
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

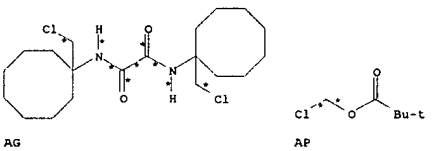
STAGE(3)
RGT E 67-56-1 MeOH

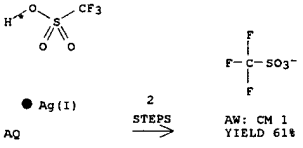
PRO AU **606970-69-8**
NTE sealed tube (2nd stage), in the dark (2nd stage)

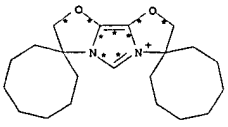
RX(72) OF 154 COMPOSED OF RX(20), RX(26)
RX(72) **AF** + AP + AQ ===> **AU**



L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)







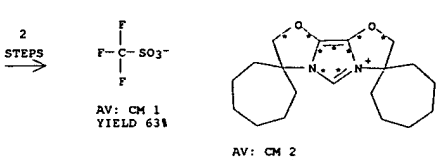
RX(21) RCT AG **814254-70-1**
RGT F 1310-73-2 NaOH
PRO AN 814254-74-5
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(27) RCT AP 18997-19-8, AQ 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT AN 814254-74-5

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(20) RCT AF **814254-69-8**
RGT F 1310-73-2 NaOH
PRO AM 814254-73-4
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(26) RCT AP 18997-19-8, AQ 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT AM 814254-73-4
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

STAGE(3)
RGT E 67-56-1 MeOH

PRO AV **814254-81-6**
NTE sealed tube (2nd stage), in the dark (2nd stage)

RX(73) OF 154 COMPOSED OF RX(21), RX(27)
RX(73) **AG** + AP + AQ ===> **AW**

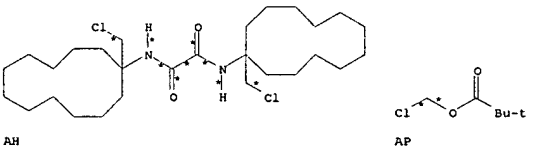
L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

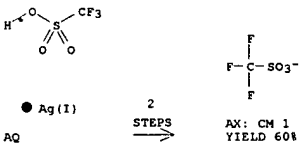
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

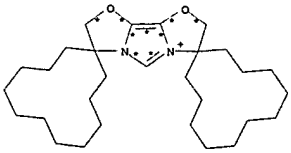
STAGE(3)
RGT E 67-56-1 MeOH

PRO AW **814254-83-6**
NTE sealed tube (2nd stage), in the dark (2nd stage)

RX(74) OF 154 COMPOSED OF RX(22), RX(28)
RX(74) **AH** + AP + AQ ===> **AX**







L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(22) RCT AH **814254-71-2**
RGT F 1310-73-2 NaOH
PRO AO 814254-75-6
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(28) RCT AP 18997-19-8, AQ 2923-28-6

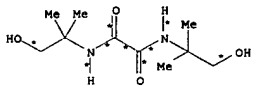
STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT AO 814254-75-6
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

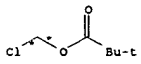
STAGE(3)
RGT E 67-56-1 MeOH

PRO AX **814254-85-8**
NTE sealed tube (2nd stage), in the dark (2nd stage)

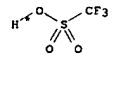
RX(99) OF 154 COMPOSED OF RX(11), RX(17), RX(23)
RX(99) R + AP + AQ ===> AR



R



AP

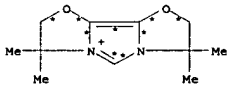


● Ag(I)

AQ

3 STEPS

AR: CM 1
YIELD 83%



AR: CM 2
YIELD 83%

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(11) RCT R **61051-10-3**

STAGE(1)
RGT AB 7719-09-7 SOCl2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, 60 deg C
SUBSTAGE(2) 3 hours, 90 deg C
SUBSTAGE(3) 90 deg C -> room temperature

STAGE(2)
RGT AC 1310-58-3 KOH
SOL 7732-18-5 Water

PRO AA 61051-14-7

RX(17) RCT AA 61051-14-7
RGT F 1310-73-2 NaOH
PRO AI 49585-66-2
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(23) RCT AP 18997-19-8, AQ 2923-28-6

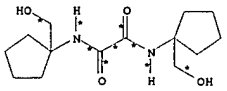
STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT AI 49585-66-2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

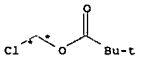
STAGE(3)
RGT E 67-56-1 MeOH

PRO AR **814254-77-8**
NTE sealed tube (2nd stage), in the dark (2nd stage)

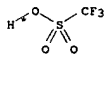
RX(101) OF 154 COMPOSED OF RX(12), RX(18), RX(24)
RX(101) T + AP + AQ ===> AT



T



AP



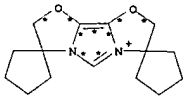
● Ag(I)

AQ

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

3 STEPS

AT: CM 1
YIELD 65%



AT: CM 2
YIELD 65%

RX(12) RCT T **814254-64-3**

STAGE(1)
RGT AB 7719-09-7 SOCl2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, 60 deg C
SUBSTAGE(2) 3 hours, 90 deg C
SUBSTAGE(3) 90 deg C -> room temperature

STAGE(2)
RGT AC 1310-58-3 KOH
SOL 7732-18-5 Water

PRO AD 814254-68-7

RX(18) RCT AD 814254-68-7
RGT F 1310-73-2 NaOH
PRO AK 814254-72-3
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(24) RCT AP 18997-19-8, AQ 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

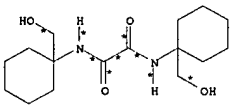
STAGE(2)
RCT AK 814254-72-3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

STAGE(3)
RGT E 67-56-1 MeOH

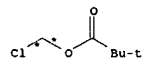
PRO AT **814254-79-0**
NTE sealed tube (2nd stage), in the dark (2nd stage)

RX(103) OF 154 COMPOSED OF RX(13), RX(19), RX(25)
RX(103) V + AP + AQ ===> AU

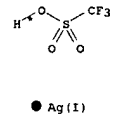
L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



V



AP

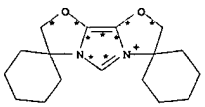


● Ag(I)

AQ

3 STEPS

AU: CM 1
YIELD 85%



AU: CM 2
YIELD 85%

RX(13) RCT V **101725-44-4**

STAGE(1)
RGT AB 7719-09-7 SOCl2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, 60 deg C
SUBSTAGE(2) 3 hours, 90 deg C
SUBSTAGE(3) 90 deg C -> room temperature

STAGE(2)
RGT AC 1310-58-3 KOH
SOL 7732-18-5 Water

PRO AE 606970-66-5

RX(19) RCT AE 606970-66-5
RGT F 1310-73-2 NaOH
PRO AL 606970-67-6
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(25) RCT AP 18997-19-8, AQ 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

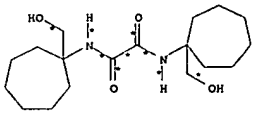
L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

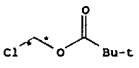
STAGE(2)
RCT AL 606970-67-6
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

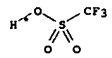
STAGE(3)
RGT E 67-56-1 MeOH

PRO AU 606970-69-8
NTE sealed tube (2nd stage), in the dark (2nd stage)

RX(105) OF 154 COMPOSED OF RX(14), RX(20), RX(26)
RX(105) X + AP + AQ ===> AV

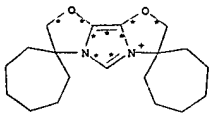

X


AP


AQ

3 STEPS


AV: CM 1
YIELD 63%


AV: CM 2
YIELD 63%

RX(14) RCT X 814254-65-4

STAGE(1)
RGT AB 7719-09-7 SOCl2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, 60 deg C
SUBSTAGE(2) 3 hours, 90 deg C
SUBSTAGE(3) 90 deg C -> room temperature

STAGE(2)
RGT AC 1310-58-3 KOH

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
SOL 7732-18-5 Water

PRO AF 814254-69-8

RX(20) RCT AF 814254-69-8
RGT F 1310-73-2 NaOH
PRO AM 814254-73-4
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(26) RCT AP 18997-19-8, AQ 2923-28-6

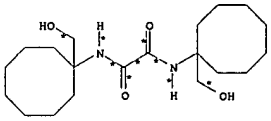
STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

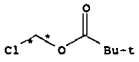
STAGE(2)
RCT AM 814254-73-4
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

STAGE(3)
RGT E 67-56-1 MeOH

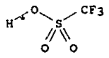
PRO AV 814254-81-4
NTE sealed tube (2nd stage), in the dark (2nd stage)

RX(107) OF 154 COMPOSED OF RX(15), RX(21), RX(27)
RX(107) Y + AP + AQ ===> AW


Y


AP

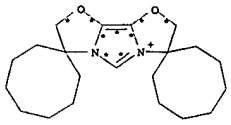
L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)


AQ

● Ag(I)

3 STEPS


AW: CM 1
YIELD 61%


AW: CM 2
YIELD 61%

RX(15) RCT Y 814254-66-5

STAGE(1)
RGT AB 7719-09-7 SOCl2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, 60 deg C
SUBSTAGE(2) 3 hours, 90 deg C
SUBSTAGE(3) 90 deg C -> room temperature

STAGE(2)
RGT AC 1310-58-3 KOH
SOL 7732-18-5 Water

PRO AG 814254-70-1

RX(21) RCT AG 814254-70-1
RGT F 1310-73-2 NaOH
PRO AN 814254-74-5
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(27) RCT AP 18997-19-8, AQ 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

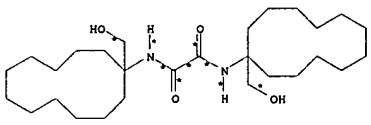
STAGE(2)

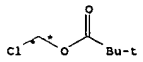
L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
RCT AN 814254-74-5
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

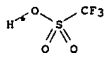
STAGE(3)
RGT E 67-56-1 MeOH

PRO AW 814254-83-6
NTE sealed tube (2nd stage), in the dark (2nd stage)

RX(109) OF 154 COMPOSED OF RX(16), RX(22), RX(28)
RX(109) Z + AP + AQ ===> AX


Z

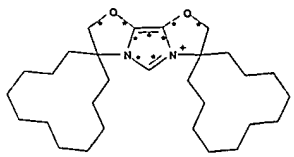

AP


AQ

● Ag(I)

3 STEPS


AX: CM 1
YIELD 60%


AX: CM 2
YIELD 60%

L62 ANSWER 8 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(16) RCT Z 814254-67-6

STAGE(1)
RGT AB 7719-09-7 SOCl2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, 60 deg C
SUBSTAGE(2) 3 hours, 90 deg C
SUBSTAGE(3) 90 deg C -> room temperature

STAGE(2)
RGT AC 1310-58-3 KOH
SOL 7732-18-5 Water

PRO AH 814254-71-2

RX(22) RCT AH 814254-71-2
RGT F 1310-73-2 NaOH
PRO AO 814254-75-6
SOL 64-17-5 EtOH, 109-99-9 THF
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 3 hours, 90 deg C

RX(28) RCT AP 18997-19-8, AQ 2923-28-6

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes, room temperature

STAGE(2)
RCT AO 814254-75-6
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 20 hours, 40 deg C
SUBSTAGE(2) 40 deg C -> room temperature

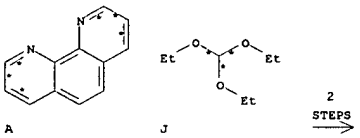
STAGE(3)
RGT E 67-56-1 MeOH

PRO AX 814254-85-8
NTE sealed tube (2nd stage), in the dark (2nd stage)

L62 ANSWER 9 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

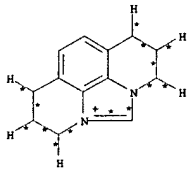
ACCESSION NUMBER: 141:395258 CASREACT
TITLE: A Benzimidazole-Based N-Heterocyclic Carbene Derived from 1,10-Phenanthroline
AUTHOR(S): Metallinos, Costa; Barrett, Fred B.; Chaytor, Jennifer
L.; Heska, Mary E. A.
CORPORATE SOURCE: Department of Chemistry, Brock University, St. Catharines, ON, L2S 3A1, Can.
SOURCE: Organic Letters (2004), 6(20), 3641-3644
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A catalytically active palladium-complexed tetracyclic N-heterocyclic carbene (NHC) was prepared in three steps from com. available 1,10-phenanthroline by using a reduction-cyclization-deprotonation sequence.
The new carbene framework is a prototype for the development of a series of chiral N-heterocyclic carbenes.
REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(10) OF 17 COMPOSED OF RX(3), RX(4)
RX(10) A + J ===> K



A J

L62 ANSWER 9 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Cl⁻

K
YIELD 89%

RX(3) RCT A 66-71-7

STAGE(1)
RGT C 25895-60-7 NaBH3CN
SOL 67-56-1 MeOH, 64-19-7 AcOH
CON SUBSTAGE(1) 0.08 hours, room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 6 hours, reflux
SUBSTAGE(4) reflux -> room temperature

STAGE(2)
RGT H 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature, pH 12

PRO G 56798-33-5
NTE optimization study, other products also detected, optimized on solvent, product depends on solvent, incremental addition of NaBH3CN

RX(4) RCT G 56798-33-5, J 122-51-0

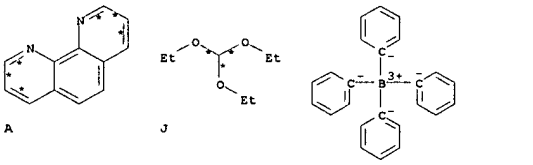
STAGE(1)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water, 122-51-0 CH(OEt)3
CON 15 hours, 80 deg C

STAGE(2)
RGT M 7782-44-7 O2
CON 2 hours, 80 deg C

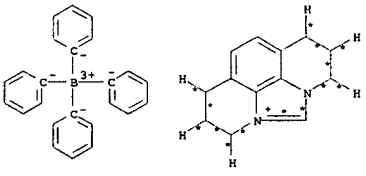
PRO K 786688-16-2

RX(15) OF 17 COMPOSED OF RX(3), RX(4), RX(8)
RX(15) A + J + AA ===> AB

L62 ANSWER 9 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



A J AA



AB: CM 1
YIELD 90%

AB: CM 2
YIELD 90%

RX(3) RCT A 66-71-7

STAGE(1)
RGT C 25895-60-7 NaBH3CN
SOL 67-56-1 MeOH, 64-19-7 AcOH
CON SUBSTAGE(1) 0.08 hours, room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 6 hours, reflux
SUBSTAGE(4) reflux -> room temperature

STAGE(2)
RGT H 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature, pH 12

PRO G 56798-33-5
NTE optimization study, other products also detected, optimized on

L62 ANSWER 9 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
solvent, product depends on solvent, incremental addition of NaBH3CN

RX(4) RCT G 56798-33-5, J 122-51-0

STAGE(1)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water, 122-51-0 CH(OEt)3
CON 15 hours, 80 deg C

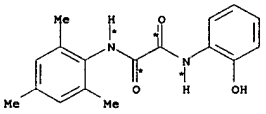
STAGE(2)
RGT M 7782-44-7 O2
CON 2 hours, 80 deg C

PRO K 786688-16-2

RX(8) RCT K 786688-16-2, AA 143-66-8
PRO AB 786688-19-5
SOL 67-56-1 MeOH
CON room temperature

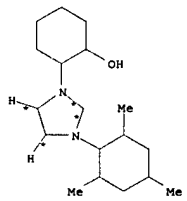
L62 ANSWER 10 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 141:140590 CASREACT
TITLE: A New Class of Chelating N-Heterocyclic Carbene Ligands and Their Complexes with Palladium
AUTHOR(S): Waltman, Andrew W.; Grubbs, Robert H.
CORPORATE SOURCE: Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, 91125, USA
SOURCE: Organometallics (2004), 23(13), 3105-3107
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new series of chelating N-(o-phenolato)-N-heterocyclic carbene (NHC) ligands mimicking salicylaldimine framework and their palladium complexes are described. General synthetic pathway to N-hydroxyaryl-substituted imidazolidinylidenes is described, starting from unsym. oxalodiamides ArHNCOCONHAr1, (2a-d) where Ar = 2,4,6-Me3C6H2 or 2,6-iPr2C6H3 (Mes and Dipp, resp.) and Ar1H = 2-HO-3-R1-5-R2C6H2 (R1, R2 = H; tBu, Me; 1-adamantyl, Me). Reduction of 2a-d followed by condensation with orthoformate gave imidazolium salts 1-Ar1-3-Ar-4,5-dihydro-1H-imidazolium chlorides (4a-d), which were converted to potassium carbenes-phenolates [ArNC3H6NAr1]-K+ and reacted with palladium dimers [Pd(PR3)MeCl]2 to give [(PR3)PdMe[ArNC3H6NAr1-κC2,κO]] (8a-d, PR3 = PPh3, PEt3). Crystal structures of complexes 8a (R1 = R2 = H; PR3 = PEt3) and 8d (R1 = 1-adamantyl, R2 = Me; PR3 = PPh3) are reported. The ligands feature a chelating phenolic unit, thereby expanding the class of available NHC ligands for organometallic catalysis.
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(11) OF 85 ...I + AG ===> AH...



I AG

L62 ANSWER 10 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Cl⁻

AH
YIELD 55%

RX(11) RCT I 724794-61-0

STAGE(1)
RGT AI 14044-65-6 BH3-THF
SOL 109-99-9 THF
CON SUBSTAGE(1) overnight, reflux
SUBSTAGE(2) reflux -> room temperature

STAGE(2)
RGT T 67-56-1 MeOH

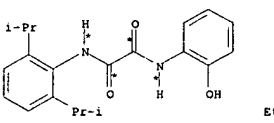
STAGE(3)
RGT N 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(4)
RCT AG 122-51-0
SOL 122-51-0 CH(OEt)3
CON SUBSTAGE(1) room temperature -> 100 deg C
SUBSTAGE(2) 6 minutes, 100 deg C

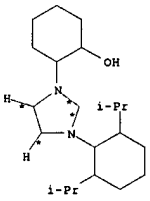
PRO AH 724794-66-5

RX(12) OF 85 ...K + AG ===> AJ...

L62 ANSWER 10 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



K AG



● Cl⁻

AJ
YIELD 85%

RX(12) RCT K 724794-62-1

STAGE(1)
RGT AI 14044-65-6 BH3-THF
SOL 109-99-9 THF
CON SUBSTAGE(1) overnight, reflux
SUBSTAGE(2) reflux -> room temperature

STAGE(2)
RGT T 67-56-1 MeOH

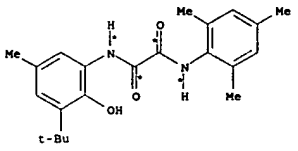
STAGE(3)
RGT N 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(4)
RCT AG 122-51-0
SOL 122-51-0 CH(OEt)3
CON SUBSTAGE(1) room temperature -> 100 deg C
SUBSTAGE(2) 6 minutes, 100 deg C

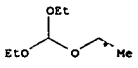
L62 ANSWER 10 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO AJ 724794-67-6

RX(13) OF 85 ...X + AG ===> AK...

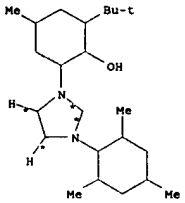


X



AG

(13)



AK
YIELD 35%

RX(13) RCT X 724794-63-2

STAGE(1)
RGT AI 14044-65-6 BH3-THF
SOL 109-99-9 THF
CON SUBSTAGE(1) overnight, reflux
SUBSTAGE(2) reflux -> room temperature

L62 ANSWER 10 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(2)
RGT T 67-56-1 MeOH

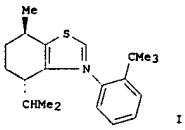
STAGE(3)
RGT N 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(4)
RCT AG 122-51-0
SOL 122-51-0 CH(OEt)3
CON SUBSTAGE(1) room temperature -> 100 deg C
SUBSTAGE(2) 6 minutes, 100 deg C

PRO AK 724794-68-7

L62 ANSWER 11 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:140358 CASREACT
TITLE: Preparation of axially chiral N,N'-diarylimidazolium and N-arylthiazolium salts and evaluation of their catalytic potential in the benzoin and in the intramolecular Stetter reactions
AUTHOR(S): Pesch, Jens; Harms, Klaus; Bach, Thorsten
CORPORATE SOURCE: Lehrstuhl fuer Organische Chemie I, Technische Universitaet Muenchen, Garching, 85747, Germany
SOURCE: European Journal of Organic Chemistry (2004), (9), 2025-2035
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



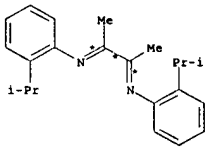
I

AB N-Aryl-substituted imidazoles were prepared which contain a stereogenic axis and which can occur as atropisomers. The di(2-isopropylphenyl)imidazolium salts could be obtained from 2-isopropylaniline and diacetyl in three steps (19% yield) whereas the synthesis of their tert-Bu analogs failed. The meso-isomer prevailed (dr = 90/10). Chiral thiazolium salts were prepared in two steps from 2-tert-butylaniline. The enantiomerically pure thiazolium salt I was obtained from α-bromomenthone and 2-tert-butylaniline (27% overall yield). In contrast to the imidazolium salts, the thiazolium salts proved to be suitable catalysts in the benzoin condensation of benzaldehyde and in the intramol. Stetter reaction of 2-OCHC6H4OCH2CH:CHCO2Me. The best results obtained with catalyst I (20 mol %) were 85% (R)-PhCOCHPhOH (40% ee) and 75% Me (R)-4-oxochroman-3-acetate. The stereogenic axis of I is not configurationally stable in the catalytically active carbene intermediate. The catalyst is recovered as a mixture of diastereomeric atropisomers in a ratio of 70:30 to 75:25.

REFERENCE COUNT: 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(20) OF 30 COMPOSED OF RX(3), RX(4)
RX(20) 2 G + 2 H ===> N

L62 ANSWER 11 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



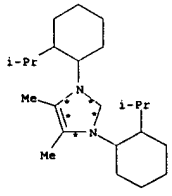
2 G

H

H

2 STEPS

N: CM 1
YIELD 45%



N: CM 2
YIELD 45%

RX(3) RCT G 49673-33-8

STAGE(1)
RGT K 7439-93-2 Li
SOL 109-99-9 THF
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT H 75-15-0
CON 20 hours, room temperature

L62 ANSWER 11 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(3)
RGT L 7732-18-5 Water

PRO I 727417-84-7, J 727417-85-8
NTE ultrasound stage 1

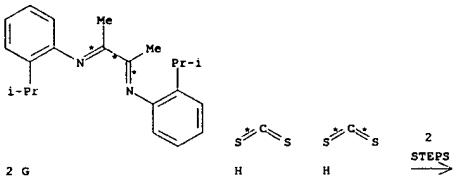
RX(4) RCT I 727417-84-7

STAGE(1)
RGT O 7601-90-3 HClO4, P 937-14-4 MCPBA
SOL 109-99-9 THF, 7732-18-5 Water
CON SUBSTAGE(1) room temperature -> -78 deg C
SUBSTAGE(2) 6 hours, -78 deg C

STAGE(2)
SOL 60-29-7 Et2O
CON 2 hours, room temperature

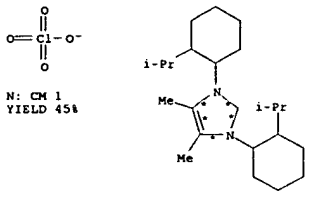
PRO N 727417-87-0
NTE stereoselective, dr for meso:dl 9:1

RX(21) OF 30 COMPOSED OF RX(3), RX(5)
RX(21) 2 G + 2 H ===> N



2 G H H

L62 ANSWER 11 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



N: CM 1
YIELD 45%

N: CM 2
YIELD 45%

RX(3) RCT G 49673-33-8

STAGE(1)
RGT K 7439-93-2 Li
SOL 109-99-9 THF
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT H 75-15-0
CON 20 hours, room temperature

STAGE(3)
RGT L 7732-18-5 Water

PRO I 727417-84-7, J 727417-85-8
NTE ultrasound stage 1

RX(5) RCT J 727417-85-8

STAGE(1)
RGT O 7601-90-3 HClO4, P 937-14-4 MCPBA
SOL 109-99-9 THF, 7732-18-5 Water
CON SUBSTAGE(1) room temperature -> -78 deg C
SUBSTAGE(2) 6 hours, -78 deg C

STAGE(2)
SOL 60-29-7 Et2O
CON 2 hours, room temperature

PRO N 727417-87-0
NTE stereoselective, dr for meso:dl 9:1

L62 ANSWER 11 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

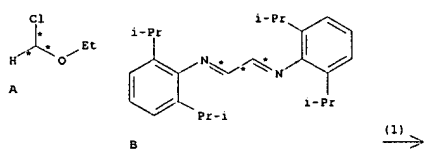
L62 ANSWER 12 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:106210 CASREACT
TITLE: Studies on high-temperature amination reactions of aromatic chlorides using discrete Palladium-N-Heterocyclic Carbene (NHC) complexes and in situ palladium/imidazolium salt protocols
AUTHOR(S): McCarroll, Andrew J.; Sandham, David A.; Titcomb, Lisa R.; Lewis, Alexandra K. de K.; Cloke, F. Geoffrey N.; Davies, Brian P.; Perez de Santana, Alejandro; Hiller, Wolfgang; Caddick, Stephen
CORPORATE SOURCE: Physics and Environmental Sciences, School of Chemistry, Chemistry Laboratory, University of Sussex, Brighton, Falmer, UK
SOURCE: Molecular Diversity (2003), 7(2-4), 115-123
CODEN: MODIF4; ISSN: 1381-1991
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The palladium catalyzed coupling of aryl chlorides and amines can be readily achieved with short reaction times when carried out at high temps. under thermal or microwave conditions. These coupling protocols are successful using two coordinate palladium-N-heterocyclic carbene complexes, or imidazolium salt protocols. Thus, Pd(dba)2/1,3-bis(diisopropylphenyl)imidazolium tetrafluoroborate catalyzed coupling reaction of 4-MeC6H4Cl with morpholine in the presence of KOBu-t in DME/DMF in microwave oven gave 97% N-(4-methylphenyl)morpholine.

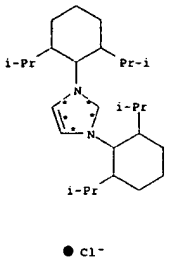
REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 17 A + B ===> C...



A B

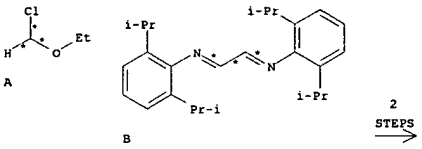
L62 ANSWER 12 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



C
YIELD 35%

RX(1) RCT A 3188-13-4, B **74663-75-5**
PRO C **250285-32-6**
CAT 7732-18-5 Water
SOL 109-99-9 THF
CON 16 hours, room temperature

RX(17) OF 17 COMPOSED OF RX(1), RX(16)
RX(17) A + B ===> S

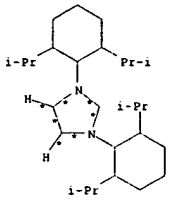


A B

2 STEPS

L62 ANSWER 12 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

S: CM 1
YIELD 98%



S: CM 2
YIELD 98%

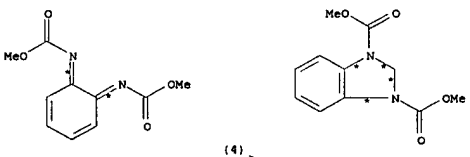
RX(1) RCT A 3188-13-4, B **74663-75-5**
PRO C 250285-32-6
CAT 7732-18-5 Water
SOL 109-99-9 THF
CON 16 hours, room temperature

RX(16) RCT C 250285-32-6
RGT AM 13826-83-0 NH4.BF4
PRO S **282109-83-5**
SOL 7732-18-5 Water
CON room temperature

L62 ANSWER 13 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 140:217168 CASREACT
TITLE: Some Heterocyclization Reactions of N,N'-Dimethoxycarbonyl-o-benzoquinone Diimine
AUTHOR(S): Velikorodov, A. V.; Babaitsev, D. D.; Mochalin, V. B.
CORPORATE SOURCE: Astrakhan State Pedagogical University, Astrakhan, 414056, Russia
SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (2003), 39(8), 1200-1201
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Diels-Alder reaction with reversed electronic requirements were reported on title compound reaction with RHC:CHR1 (R = C6H5; R1 = H; RR1 = CH:CHCH2, CH2CH2CH2CH2).
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(4) OF 4 I + B ===> J

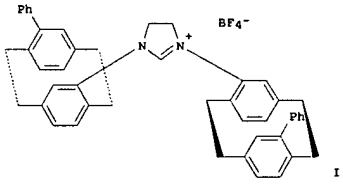
I



B (4) J
YIELD 87%

RX(4) RCT I 2932-82-3, B **139499-83-5**
PRO J **664333-94-2**
SOL 67-66-3 CHCl3, 60-29-7 Et2O
CON 1 hour, 0 - 5 deg C

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 140:181180 CASREACT
TITLE: Asymmetric addition of aryl boron reagents to enones with rhodium dicyclophane imidazolium carbene catalysis
AUTHOR(S): Ma, Yudao; Song, Chun; Ma, Changqing; Sun, Zhijun; Chai, Qiang; Andrus, Merritt B.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602-5700, USA
SOURCE: Angewandte Chemie, International Edition (2003), 42(47), 5871-5874
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

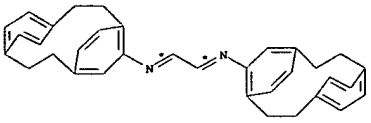


I

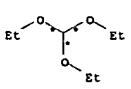
AB Chiral dicyclophane imidazoliumcarbene ligands, e.g., I, were prepared and screened as catalyst in addition reaction of cyclohexenone and arylboronic acids in the presence of rhodium. It was found that the ligand with 2-methoxyphenyl substituents on the dicyclophane gave the highest enantiomeric excess and isolation yield. The catalyst was used effectively in asym. conjugate addition of alkenones with arylboron reagents to yield chiral ketones in high yield.
REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(60) OF 91 COMPOSED OF RX(35), RX(36)
RX(60) BE + N ===> BG

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



BE



N

2
STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(35) RCT BE **658711-12-7**

STAGE(1)
RGT P 16940-66-2 NaBH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 1 hour, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 16 hours, room temperature
SUBSTAGE(4) 3 hours, reflux
SUBSTAGE(5) reflux -> room temperature

STAGE(2)
RGT Q 7732-18-5 Water
CON 0.5 hours

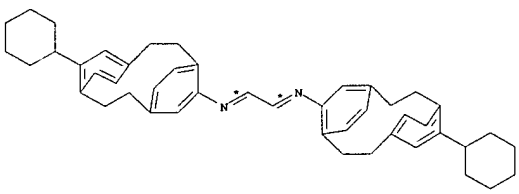
STAGE(3)
RGT R 7647-01-0 HCl

PRO BF 658711-13-8

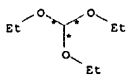
RX(36) RCT BF 658711-13-8, N 122-51-0
PRO BG **658712-03-9**
CAT 64-18-6 HCO2H
CON SUBSTAGE(1) 60 hours, reflux
SUBSTAGE(2) reflux -> room temperature

RX(65) OF 91 COMPOSED OF RX(40), RX(43)
RX(65) **BH** + N ===> **BN**

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



BI



N

2
STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A

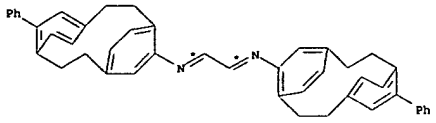
● Cl⁻

BO
YIELD 90%

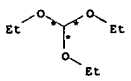
RX(41) RCT BI **658711-15-0**

STAGE(1)
RGT P 16940-66-2 NaBH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 1 hour, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 16 hours, room temperature
SUBSTAGE(4) 3 hours, reflux

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



BH



N

2
STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(40) RCT BH **658711-14-9**

STAGE(1)
RGT P 16940-66-2 NaBH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 1 hour, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 16 hours, room temperature
SUBSTAGE(4) 3 hours, reflux
SUBSTAGE(5) reflux -> room temperature

STAGE(2)
RGT Q 7732-18-5 Water
CON 0.5 hours

STAGE(3)
RGT R 7647-01-0 HCl

PRO BK 658711-17-2

RX(43) RCT BK 658711-17-2, N 122-51-0
PRO BN **658712-06-2**
CAT 64-18-6 HCO2H
CON SUBSTAGE(1) 60 hours, reflux
SUBSTAGE(2) reflux -> room temperature

RX(66) OF 91 COMPOSED OF RX(41), RX(44)
RX(66) **BI** + N ===> **BO**

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
SUBSTAGE(5) reflux -> room temperature

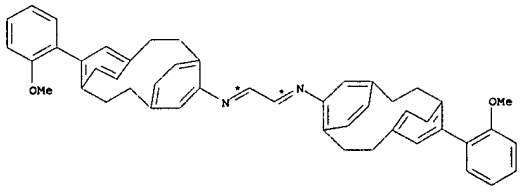
STAGE(2)
RGT Q 7732-18-5 Water
CON 0.5 hours

STAGE(3)
RGT R 7647-01-0 HCl

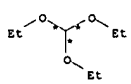
PRO BL 658711-18-3

RX(44) RCT BL 658711-18-3, N 122-51-0
PRO BO **658712-09-5**
CAT 64-18-6 HCO2H
CON SUBSTAGE(1) 60 hours, reflux
SUBSTAGE(2) reflux -> room temperature

RX(67) OF 91 COMPOSED OF RX(42), RX(45)
RX(67) **BJ** + N ===> **BP**



BJ



N

2
STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

● Cl⁻

BP
YIELD 90%

RX(42) RCT BJ **658711-16-1**

STAGE(1)
RGT P 16940-66-2 NaBH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 1 hour, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 16 hours, room temperature
SUBSTAGE(4) 3 hours, reflux
SUBSTAGE(5) reflux -> room temperature

STAGE(2)
RGT Q 7732-18-5 Water
CON 0.5 hours

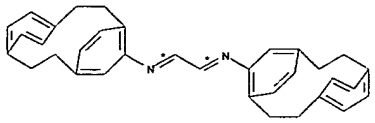
STAGE(3)
RGT R 7647-01-0 HCl

PRO BM 658711-19-4

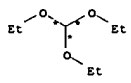
RX(45) RCT BM 658711-19-4, N 122-51-0
PRO BP **658712-11-9**
CAT 64-18-6 HCO2H
CON SUBSTAGE(1) 60 hours, reflux
SUBSTAGE(2) reflux -> room temperature

RX(75) OF 91 COMPOSED OF RX(35), RX(36), RX(52)
RX(75) **BE** + N ===> O

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



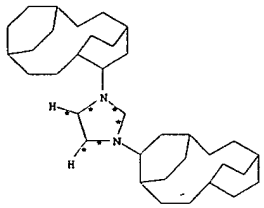
BE



N

3 STEPS

O: CM 1



O: CM 2

RX(35) RCT BE **658711-12-7**

STAGE(1)
RGT P 16940-66-2 NaBH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 1 hour, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 16 hours, room temperature
SUBSTAGE(4) 3 hours, reflux
SUBSTAGE(5) reflux -> room temperature

STAGE(2)
RGT Q 7732-18-5 Water
CON 0.5 hours

STAGE(3)
RGT R 7647-01-0 HCl

PRO BF 658711-13-8

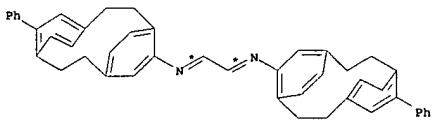
RX(36) RCT BF 658711-13-8, N 122-51-0

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

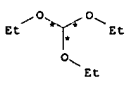
PRO BG 658712-03-9
CAT 64-18-6 HCO2H
CON SUBSTAGE(1) 60 hours, reflux
SUBSTAGE(2) reflux -> room temperature

RX(52) RCT BG 658712-03-9
RGT S 13826-83-0 NH4.BF4
PRO O **658711-04-7**
SOL 67-56-1 MeOH
CON SUBSTAGE(1) 3 hours, reflux
SUBSTAGE(2) reflux -> room temperature

RX(83) OF 91 COMPOSED OF RX(40), RX(43), RX(46)
RX(83) **BH** + N ===> W



BH

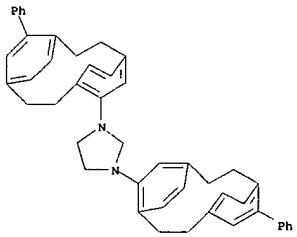


N

3 STEPS

W: CM 1

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



W: CM 2

RX(40) RCT BH **658711-14-9**

STAGE(1)
RGT P 16940-66-2 NaBH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 1 hour, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 16 hours, room temperature
SUBSTAGE(4) 3 hours, reflux
SUBSTAGE(5) reflux -> room temperature

STAGE(2)
RGT Q 7732-18-5 Water
CON 0.5 hours

STAGE(3)
RGT R 7647-01-0 HCl

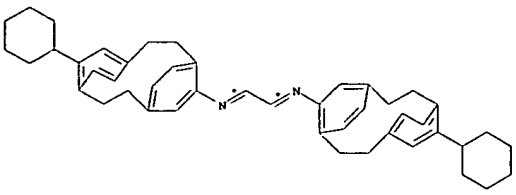
PRO BK 658711-17-2

RX(43) RCT BK 658711-17-2, N 122-51-0
PRO BN 658712-06-2
CAT 64-18-6 HCO2H
CON SUBSTAGE(1) 60 hours, reflux
SUBSTAGE(2) reflux -> room temperature

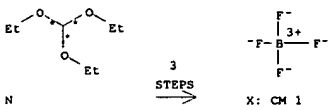
RX(46) RCT BN 658712-06-2
RGT S 13826-83-0 NH4.BF4
PRO W **658711-06-9**
SOL 67-56-1 MeOH
CON SUBSTAGE(1) 3 hours, reflux
SUBSTAGE(2) reflux -> room temperature

RX(85) OF 91 COMPOSED OF RX(41), RX(44), RX(47)
RX(85) **BI** + N ===> X

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



BI



N X: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A

X: CM 2

RX(41) RCT BI 658711-15-0

STAGE(1)
RGT P 16940-66-2 NaBH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 1 hour, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 16 hours, room temperature
SUBSTAGE(4) 3 hours, reflux
SUBSTAGE(5) reflux -> room temperature

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A

Y: CM 2

RX(42) RCT BJ 658711-16-1

STAGE(1)
RGT P 16940-66-2 NaBH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 1 hour, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 16 hours, room temperature
SUBSTAGE(4) 3 hours, reflux
SUBSTAGE(5) reflux -> room temperature

STAGE(2)
RGT Q 7732-18-5 Water
CON 0.5 hours

STAGE(3)
RGT R 7647-01-0 HCl

PRO BM 658711-19-4

RX(45) RCT BM 658711-19-4, N 122-51-0
PRO BP 658712-11-9
CAT 64-18-6 HCO2H
CON SUBSTAGE(1) 60 hours, reflux
SUBSTAGE(2) reflux -> room temperature

RX(48) RCT BP 658712-11-9
RGT S 13826-83-0 NH4.BF4
PRO Y 658711-10-5
SOL 67-56-1 MeOH
CON SUBSTAGE(1) 3 hours, reflux
SUBSTAGE(2) reflux -> room temperature

L62 ANSWER 14 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(2)
RGT Q 7732-18-5 Water
CON 0.5 hours

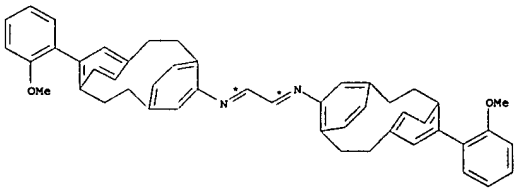
STAGE(3)
RGT R 7647-01-0 HCl

PRO BL 658711-18-3

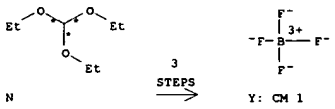
RX(44) RCT BL 658711-18-3, N 122-51-0
PRO BO 658712-09-5
CAT 64-18-6 HCO2H
CON SUBSTAGE(1) 60 hours, reflux
SUBSTAGE(2) reflux -> room temperature

RX(47) RCT BO 658712-09-5
RGT S 13826-83-0 NH4.BF4
PRO X 658711-08-1
SOL 67-56-1 MeOH
CON SUBSTAGE(1) 3 hours, reflux
SUBSTAGE(2) reflux -> room temperature

RX(87) OF 91 COMPOSED OF RX(42), RX(45), RX(48)
RX(87) BJ + N ===> Y



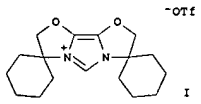
BJ



N Y: CM 1

L62 ANSWER 15 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

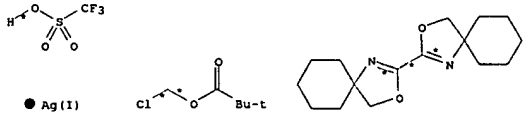
ACCESSION NUMBER: 139:276684 CASREACT
TITLE: An N-heterocyclic carbene ligand with flexible steric bulk allows Suzuki cross-coupling of sterically hindered aryl chlorides at room temperature
AUTHOR(S): Altenhoff, Goreon; Goddard, Richard; Lehmann, Christian W.; Glorius, Frank
CORPORATE SOURCE: Max-Planck-Institut fuer Kohlenforschung, Muelheim an der Ruhr, 45470, Germany
SOURCE: Angewandte Chemie, International Edition (2003), 42(31), 3690-3693
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A catalyst prepared from Pd(OAc)2 and imidazolium salt I catalyzed the Suzuki cross-coupling of sterically hindered and unhindered, activated and unactivated, aryl chlorides and aryl boronic acids. Obtained were di- and tri-ortho-substituted biphenyl compds.
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(4) OF 23 ...L + M + H ===> N

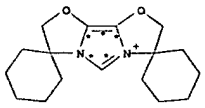


L M H

L62 ANSWER 15 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

(4) ⟹

N: CM 1
YIELD 85%



N: CM 2
YIELD 85%

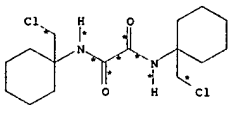
RX(4) RCT L 2923-28-6, M 18997-19-8

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes

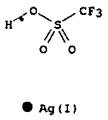
STAGE(2)
RCT H 606970-67-6
CON 20 hours, 40 deg C

PRO N 606970-69-8
NTE in the dark second stage

RX(20) OF 23 COMPOSED OF RX(3), RX(4)
RX(20) F + L + M ===> N

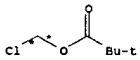


F



● Ag(I)

L

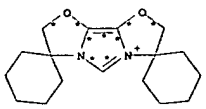


M

L62 ANSWER 15 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

2 STEPS ⟹

N: CM 1
YIELD 85%



N: CM 2
YIELD 85%

RX(3) RCT F 606970-66-5
RGT I 1310-73-2 NaOH
PRO H 606970-67-6
SOL 109-99-9 THF, 64-17-5 EtOH
CON SUBSTAGE(1) 20 minutes, room temperature
SUBSTAGE(2) room temperature -> 80 deg C
SUBSTAGE(3) 1.5 hours, 80 deg C

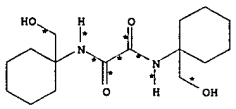
RX(4) RCT L 2923-28-6, M 18997-19-8

STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes

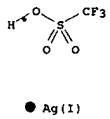
STAGE(2)
RCT H 606970-67-6
CON 20 hours, 40 deg C

PRO N 606970-69-8
NTE in the dark second stage

RX(22) OF 23 COMPOSED OF RX(2), RX(3), RX(4)
RX(22) C + L + M ===> N

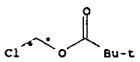


C



● Ag(I)

L

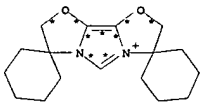


M

L62 ANSWER 15 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

3 STEPS ⟹

N: CM 1
YIELD 85%



N: CM 2
YIELD 85%

RX(2) RCT C 101725-44-4
RGT G 7719-09-7 SOCl2
PRO F 606970-66-5
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 1 hour, 60 deg C
SUBSTAGE(2) 3 hours, 90 deg C

RX(3) RCT F 606970-66-5
RGT I 1310-73-2 NaOH
PRO H 606970-67-6
SOL 109-99-9 THF, 64-17-5 EtOH
CON SUBSTAGE(1) 20 minutes, room temperature
SUBSTAGE(2) room temperature -> 80 deg C
SUBSTAGE(3) 1.5 hours, 80 deg C

RX(4) RCT L 2923-28-6, M 18997-19-8

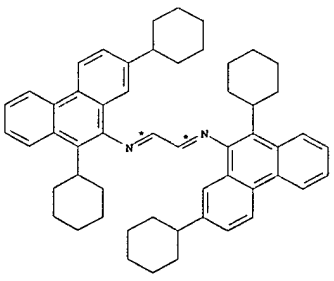
STAGE(1)
SOL 75-09-2 CH2Cl2
CON 45 minutes

STAGE(2)
RCT H 606970-67-6
CON 20 hours, 40 deg C

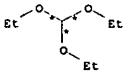
PRO N 606970-69-8
NTE in the dark second stage

L62 ANSWER 16 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 139:276460 CASREACT
TITLE: Sonogashira Coupling Using Bulky Palladium-Phenanthryl Imidazolium Carbene Catalysis
AUTHOR(S): Ma, Yudao; Song, Chun; Jiang, Wei; Wu, Quansheng; Wang, Yong; Liu, Xueying; Andrus, Merritt B.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602-5700, USA
SOURCE: Organic Letters (2003), 5(18), 3317-3319
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bulky phenanthrenyl imidazolium-derived carbene ligands were investigated for copper-free Sonogashira coupling with terminal acetylenes. Aryl bromides and iodides gave coupled products in excellent yields from the Pd(PPh3)2Cl2 complex with potassium t-butoxide and 18-crown-6 in THF. A remarkable dependence on the size of the ligand was found. The highest yields were obtained with the bulky (2,9-dicyclohexyl-10-phenanthrenyl)imidazolylidene ligand.
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(53) OF 74 COMPOSED OF RX(44), RX(37)
RX(53) CE + BG ===> G

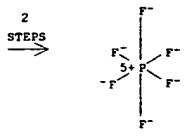


CE



BG

L62 ANSWER 16 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



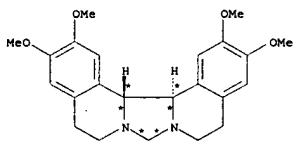
G: CM 1
YIELD 96%

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(44) RCT CE **605686-25-7**
RGT CH 16940-66-2 NaBH4
PRO BF 605686-26-8
SOL 109-99-9 THF
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 1 hour, 0 deg C
SUBSTAGE(3) 0 deg C -> room temperature
SUBSTAGE(4) 16 hours, room temperature
SUBSTAGE(5) 3 hours, reflux

RX(37) RCT BF 605686-26-8, BG 122-51-0
PRO G **605686-20-2**
CAT 64-18-6 HCO2H
CON 60 hours, reflux

L62 ANSWER 17 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



AT
YIELD 94%

RX(14)

STAGE(1)
RGT AQ 1148-11-4 1,2-Pyrrolidinedicarboxylic acid, 1-(phenylmethyl) ester, (2S)-, AR 25895-60-7 NaBH3CN
SOL 109-99-9 THF
CON 0 deg C

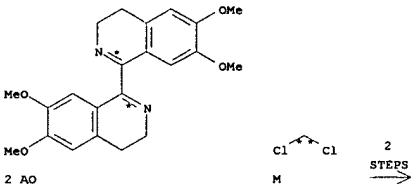
STAGE(2)
RCT AO **30340-61-5**
SOL 109-99-9 THF
CON SUBSTAGE(1) -25 deg C
SUBSTAGE(2) 15 hours, -25 deg C -> room temperature

PRO B 75370-82-0, AP 75370-78-4
NTE 82% overall yield

RX(15) RCT M 75-09-2, B 75370-82-0
RGT P 584-08-7 K2CO3
PRO AT **75370-84-2**
CON 3 days, reflux

L62 ANSWER 17 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 139:6825 CASREACT
TITLE: New N-acyl, N-alkyl, and N-bridged derivatives of rac-6,6',7,7'-tetramethoxy-1,1',2,2',3,3',4,4'-octahydro-1,1'-bisisoquinoline
AUTHOR(S): Busato, Stephan; Craig, Donald C.; Judeh, Zaher M. A.; Read, Roger W.
CORPORATE SOURCE: School of Chemical Sciences, The University of New South Wales, Sydney, 2052, Australia
SOURCE: Tetrahedron (2003), 59(4), 461-472
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The preparation of potential new ligand systems based on the rac-1,1',2,2',3,3',4,4'-octahydro-6,6',7,7'-tetramethoxy-1,1'-bisisoquinoline skeleton has been investigated. Syntheses of N-(2-bromobenzyl), N-(3-acetoxybenzyl), N-acetyl, N-chloroacetyl, N-chlorocarbonyl, N-ethoxycarbonyl and N-tert-butyloxycarbonyl derivs. and five macrocyclic, polyether containing derivs. are also described. Asym. reduction of one of the bisamine compound is also reported. Crystal structure of some of the products were also investigated.
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

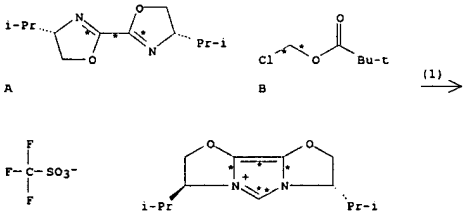
RX(44) OF 52 COMPOSED OF RX(14), RX(15)
RX(44) 2 **AO** + **M** ===> **AT**



2 AO M

L62 ANSWER 18 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 138:321365 CASREACT
TITLE: Oxazolines as chiral building blocks for imidazolium salts and N-heterocyclic carbene ligands
AUTHOR(S): Glorius, Frank; Altenhoff, Gereon; Goddard, Richard; Lehmann, Christian
CORPORATE SOURCE: Max-Planck-Institut fuer Kohlenforschung, Muelheim/Ruhr, 45470, Germany
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (22), 2704-2705
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Enantiomerically pure imidazolium triflates can be readily prepared from bioxazolines and oxazolineimines. Deprotonation of imidazolium triflate gives a chiral N-heterocyclic carbene that can act as a ligand in a catalytically active palladium complex.
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 13 **A** + **B** ===> **C**...



A B

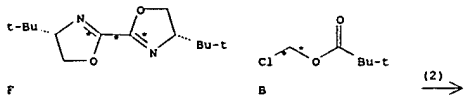
C: CM 1
YIELD 80%

C: CM 2
YIELD 80%

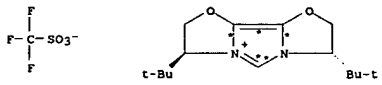
RX(1) RCT A **131833-89-1**, B 18997-19-8
RGT D 2923-28-6 AgO3SCF3
PRO C **512193-98-5**
SOL 75-09-2 CH2Cl2
CON 24 hours, 40 deg C
NTE in the dark

RX(2) OF 13 **F** + **B** ===> **G**

L62 ANSWER 18 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



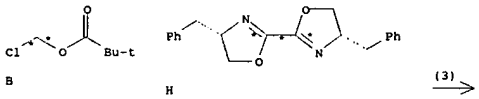
F B



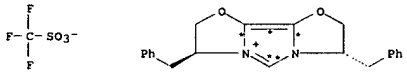
G: CM 1 G: CM 2
YIELD 75% YIELD 75%

RX(2) RCT F 135565-31-0, B 18997-19-8
RGT D 2923-28-6 AgO3SCF3
PRO G 512194-01-3
SOL 75-09-2 CH2Cl2
CON 24 hours, 40 deg C
NTE in the dark

RX(3) OF 13 B + H ===> I



B H



I: CM 1 I: CM 2
YIELD 36% YIELD 36%

RX(3) RCT B 18997-19-8

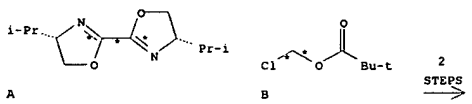
L62 ANSWER 18 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(1)
RGT D 2923-28-6 AgO3SCF3
SOL 75-09-2 CH2Cl2
CON 1 hour

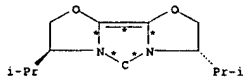
STAGE(2)
RCT H 133463-88-4
CON 24 hours, 40 deg C

PRO I 512194-04-6
NTE in the dark

RX(12) OF 13 COMPOSED OF RX(1), RX(8)
RX(12) A + B ===> AC



A B

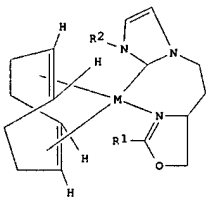


AC

RX(1) RCT A 131833-89-1, B 18997-19-8
RGT D 2923-28-6 AgO3SCF3
PRO C 512193-98-5
SOL 75-09-2 CH2Cl2
CON 24 hours, 40 deg C
NTE in the dark

RX(8) RCT C 512193-98-5
RGT AD 7693-26-7 KH
PRO AC 512194-17-1
CAT 865-47-4 t-BuOK
SOL 109-99-9 THF
CON room temperature

L62 ANSWER 19 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 138:170340 CASREACT
TITLE: Optically Active Iridium Imidazol-2-ylidene-oxazoline Complexes: Preparation and Use in Asymmetric Hydrogenation of Arylalkenes
AUTHOR(S): Perry, Marc C.; Cui, Xiuhua; Powell, Mark T.; Hou, Duen-Ren; Reibenspies, Joseph H.; Burgess, Kevin
CORPORATE SOURCE: Chemistry Department, Texas A M University, College Station, TX, 77842, USA
SOURCE: Journal of the American Chemical Society (2003), 125(1), 113-123
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

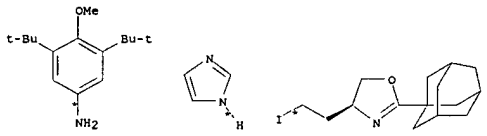


I

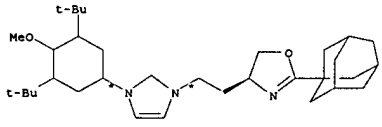
AB A library of iridium imidazolylidene oxazoline complexes [I; wherein M = Ir; R1 = 1-Ad, t-Bu, CHPh2, Ph, etc.; R2 = t-Bu, CHPh2, Cy, 2,4,6-Me3C6H2, 3,5-t-Bu2-4-MeOC6H2, 2,5-Et2C6H3, 2,6-i-Pr2-C6H3, 2,5-t-Bu2-C6H3, 1-Ad, etc.] were prepared and used as catalysts in asym. hydrogenations of arylalkenes. Three of the complexes [M = Ir; R1 = 1-Ad, R2 = t-Bu (5ab); R1 = 1-Ad, R2 = Cy (5ad); R1 = Ph, R2 = 2,6-i-Pr2-C6H3 (5dp)] and a similar rhodium complex [M = Rh; R1 = 1-Ad, R2 = 2,6-i-Pr2-C6H3 (6ap)] were studied by single-crystal x-ray diffraction techniques. This revealed mol. features of 6ap, and presumably the corresponding iridium complex 5ap, that the others do not have. In enantioselective hydrogenations of arylalkenes complex 5ap was the best for many, but not all, substrates. The enantioselectivities and conversions observed were sensitive to minor changes to the catalyst and substrate structure. Ligands with aliphatic N-heterocyclic carbene substituents gave complexes that are inactive, and do not lose the 1,5-cyclooctadiene ligands under the hydrogenation conditions. Expts. to investigate this unexpected observation imply that it is of a steric, rather than an electronic, origin. Temperature and pressure effects on the conversions and enantioselectivities of these reactions had minimal effects for some alkenes, but profound effects for others. In one case, the enantioselectivities obtained at high-pressure/low-temperature conditions were opposite to those obtained under high-temperature/low-pressure conditions (-64% enantiomeric excess vs. +89% enantiomeric excess); a transformation from one prevalent mechanism to another is inferred from this. The studies of pressure dependence revealed that many reactions proceeded with high conversions, and optimal enantioselectivities in approx. 2 h when only 1 bar of hydrogen was used. Deuterium-labeling expts. provide evidence for other types of competing mechanisms that lead to D-incorporation at positions that do not correspond to direct addn. to the double bond.
REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 19 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(67) OF 143 COMPOSED OF RX(14), RX(22)
RX(67) AP + AF + BH ===> BL



AP AF BH



BL

RX(14) RCT AP 343217-35-6, AF 288-32-4

STAGE(1)
RGT AH 534-17-8 Cs2CO3, AI 538-58-9 1,4-Pentadien-3-one, 1,5-diphenyl-, AJ 66-71-7 1,10-Phenanthroline, AK

L62 ANSWER 19 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

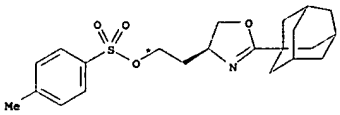
42152-44-3 Cuprous triflate
SOL 1330-20-7 Xylene
CON SUBSTAGE(1) 36 hours, 125 deg C
SUBSTAGE(2) 125 deg C -> room temperature

STAGE(2)
RGT F 12125-02-9 NH4Cl
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

PRO AQ 496067-55-1

RX(22) RCT AQ 496067-55-1, BH 369657-19-2
PRO BL 496067-64-2
SOL 68-12-2 DMF
CON 12 hours, 80 deg C
NTE stereoselective

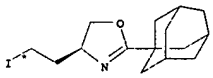
RX(108) OF 143 COMPOSED OF REACTION SEQUENCE RX(28), RX(22)
AND REACTION SEQUENCE RX(14), RX(22)
...BV ===> BH...
...AP + AF + BH ===> BL



Me

BV

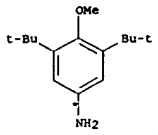
2
STEPS



BH

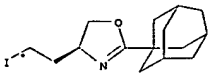
START NEXT REACTION SEQUENCE

L62 ANSWER 19 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



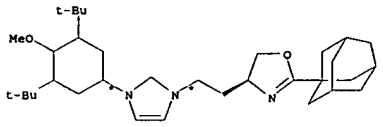
AP

AF



BH

2
STEPS



BL

RX(28) RCT BV 369657-20-5
RGT BW 7681-11-0 KI
PRO BH 369657-19-2
SOL 67-64-1 Me2CO
CON 4 hours, 55 deg C

RX(14) RCT AP 343217-35-6, AF 288-32-4

STAGE(1)
RGT AH 534-17-8 Cs2CO3, AI 538-58-9 1,4-Pentadien-3-one, 1,5-diphenyl-, AJ 66-71-7 1,10-Phenanthroline, AK 42152-44-3 Cuprous triflate
SOL 1330-20-7 Xylene
CON SUBSTAGE(1) 36 hours, 125 deg C
SUBSTAGE(2) 125 deg C -> room temperature

L62 ANSWER 19 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(2)
RGT F 12125-02-9 NH4Cl
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

PRO AQ 496067-55-1

RX(22) RCT AQ 496067-55-1, BH 369657-19-2
PRO BL 496067-64-2
SOL 68-12-2 DMF
CON 12 hours, 80 deg C
NTE stereoselective

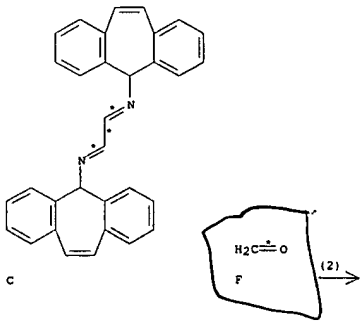
L62 ANSWER 20 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 138:137376 CASREACT
TITLE: Synthesis of a transient tropylidene substituted N-heterocyclic carbene (tropNHC): rearrangement and formation of its gold complex
AUTHOR(S): Boehler, Carsten; Stein, Daniel; Donati, Nicola; Gruetzmacher, Hansjoerg
CORPORATE SOURCE: Department of Chemistry, Laboratory of Inorganic Chemistry, ETH-Hoenggerberg, Zurich, CH-8093, Switz.
SOURCE: New Journal of Chemistry (2002), 26(10), 1291-1295
CODEN: NJCHE5; ISSN: 1144-0546
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The condensation reaction of the primary tropylidenyl amine tropamine RNH2 (2, R = 5H-dibenzo[a,d]cyclohepten-5-yl) with glyoxal 3 leads to the corresponding 1,4-diazadiene bistropdad RN:CHCH:NR (4) in high yield. With formaldehyde and ethereal HCl, 4 is transformed to the bistropimidazolium salt 1,3-R2-imidazolium chloride (5). Deprotonation with KOtBu in THF did not gave a stable N-heterocyclic carbene bistropNHC 1,3-R2-imidazol-2-ylidene (6), but the imidazole derivative 2-(5H-dibenzo[a,d]cyclohepten-10-yl)-1-R-1H-imidazole 9 as a product of a rearrangement. However, the unstable carbene 6 can be trapped when it is generated in the presence of [AuCl(PPh3)] whereby the stable cationic mixed phosphine carbene gold complex [(1,3-R2-imidazol-2-ylidene)(PPh3)Au]Cl (10) was obtained and characterized by x-ray diffraction.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 9 ...C + F ===> G...

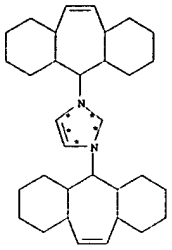


C

F

(2)

L62 ANSWER 20 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



G
YIELD 79%

RX(2) RCT C 492446-84-1, F 50-00-0

STAGE(1)
SOL 108-88-3 PhMe
CON room temperature

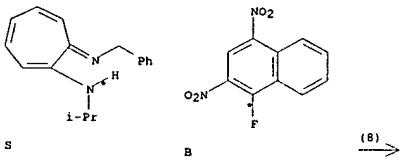
STAGE(2)
RGT H 7647-01-0 HCl
SOL 60-29-7 Et2O
CON 2 days, room temperature

PRO G 492446-85-2
NTE paraformaldehyde was used

L62 ANSWER 21 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 138:136761 CASREACT
TITLE: Acylotropic Tautomerism: XXXV. R.dblarw.L-Inversion of Configuration of Dipolar Spyrocyclic and Open-Chain 2-Arylaminotropone Isomers
AUTHOR(S): Olekhnovich, L. P.; Budarina, Z. N.; Borodkin, G. S.; Kurbatov, S. V.; Vaslyaeva, G. S.; Zhdanov, Yu. A.
CORPORATE SOURCE: Rostov State University, Rostov-on-Don, 344090, Russia
SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (2002), 38(5), 713-722
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
AB R.dblarw.L-Inversion of chiral spirocyclic and open-chain 2-arylaminotropone derivs. with varied heteroatom (O, S, N) was studied. Kinetic relations holding in the RL-permutation are discussed. Its mechanism includes formation and dissociation of spiro bonds and torsion stereodynamics.
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

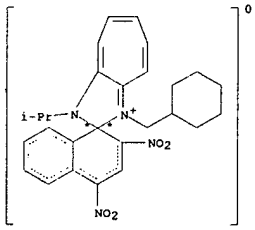
VERIFICATION INCOMPLETE

RX(8) OF 35 ...S + B ===> T



S B (8)

L62 ANSWER 21 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

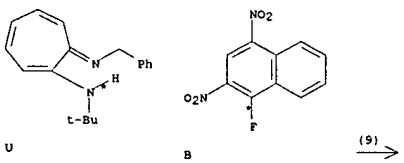


T
YIELD 66%

RX(8) RCT S 491879-92-6, B 954-50-7
PRO T 492435-83-3
SOL 67-66-3 CHCl3
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) reflux -> 80 deg C
SUBSTAGE(3) 6 - 8 hours, 80 deg C

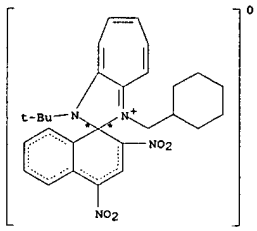
VERIFICATION INCOMPLETE

RX(9) OF 35 ...U + B ===> V



U B (9)

L62 ANSWER 21 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



V
YIELD 78%

RX(9) RCT U 491879-91-5, B 954-50-7
PRO V 492435-84-4
SOL 67-66-3 CHCl3
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) reflux -> 80 deg C
SUBSTAGE(3) 6 - 8 hours, 80 deg C

L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 137:353285 CASREACT
TITLE: Convenient synthesis of human calcitonin and its methionine sulfoxide derivative
AUTHOR(S): Shi, Tiesheng; Rabenstein, Dallas L.
CORPORATE SOURCE: Department of Chemistry, University of California, Riverside, CA, 92521, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(16), 2237-2240
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The human calcitonin peptide chain was assembled using Fmoc solid-phase peptide synthesis chemical The combinations of cleavage Reagent H (TFA 81%, phenol 5%, thioanisole 5%, ethanedithiol 2.5%, dimethylsulfide 2%, water 3%, ammonium iodide 1.5 %) with trans-[Pt(en)2Cl2]2+ and Reagents B (TFA 88%, phenol 5%, triisopropylsilane 2%,and water 5%), K (TFA 82.5%, phenol 5%, thioanisole 5%, ethanedithiol 2.5%, and water 5%), and R (TFA 90%, thioanisole 5%, ethanedithiol 3%, anisole 2%) with trans-[Pt(CN)4Cl2]2- provide convenient methods for the synthesis of human calcitonin and its methionine sulfoxide derivative; the formation of intramol. disulfide bonds by the above Pt(IV) oxidants is essentially quant.

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

VERIFICATION INCOMPLETE

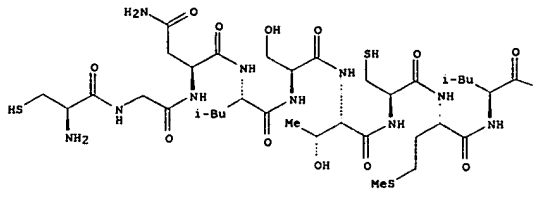
RX(40) OF 40 COMPOSED OF REACTION SEQUENCE RX(1), RX(3), RX(6)
AND REACTION SEQUENCE RX(2), RX(3), RX(6)
AND REACTION SEQUENCE RX(2), RX(4), RX(6)
AND REACTION SEQUENCE RX(1), RX(4), RX(6)

...A + B + C + D + E + F + G + H + I + J + K + L + M +
N + O + P + Q + X ===> Y...
...A + B + C + D + E + F + G + H + I + J + K + L + M +
N + W + P + Q ===> X...
...A + B + C + D + E + F + G + H + I + J + K + L + M +
N + W + P + Q ===> X...
...A + B + C + D + E + F + G + H + I + J + K + L + M +
N + O + P + Q + X + Y ===> AH

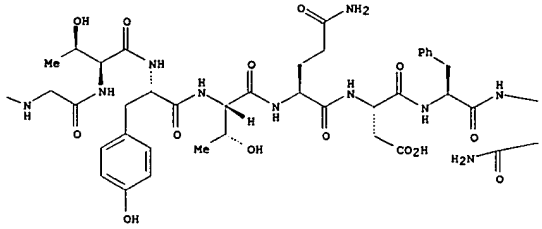
3 STEPS

L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



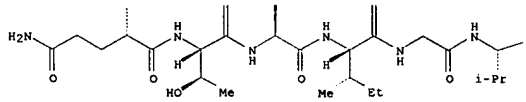
PAGE 1-B



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

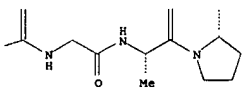
PAGE 2-C



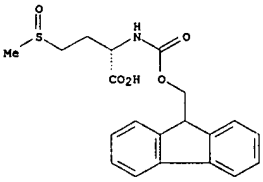
L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

START NEXT REACTION SEQUENCE

PAGE 2-D



Y



2 W

3 STEPS

START NEXT REACTION SEQUENCE

STRUCTURE DIAGRAM IS NOT AVAILABLE

3 STEPS

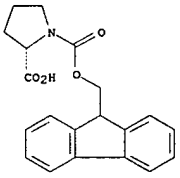
X

STRUCTURE DIAGRAM IS NOT AVAILABLE

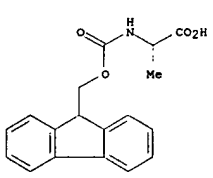
X

START NEXT REACTION SEQUENCE

L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



4 A



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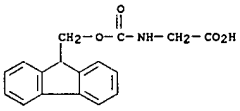

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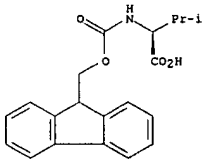

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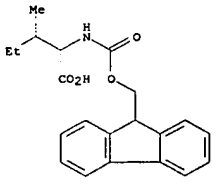

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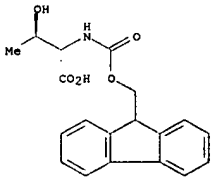
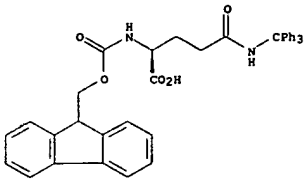
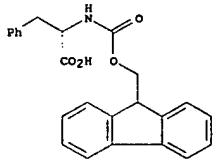


4 F

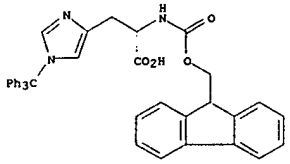
L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



4 G



4 H



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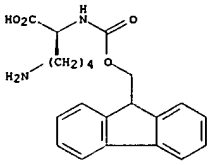

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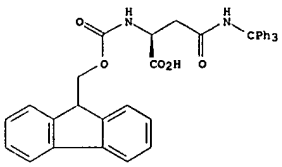
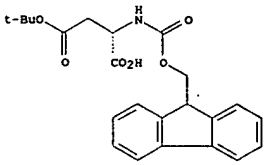


4 K

L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



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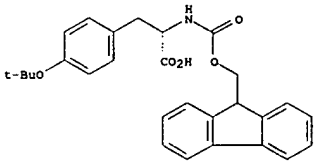
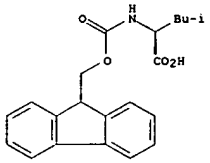


4 M



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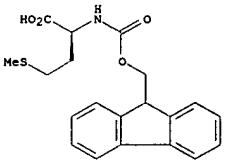

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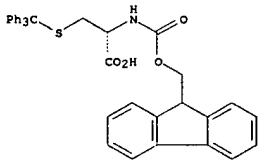

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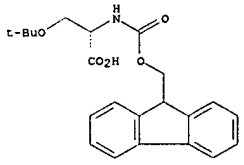
L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



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STRUCTURE DIAGRAM IS NOT AVAILABLE

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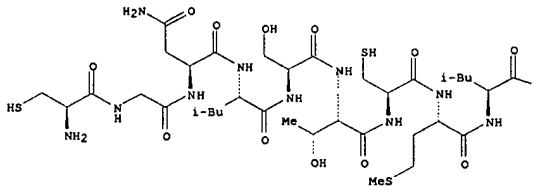
PAGE 1-A



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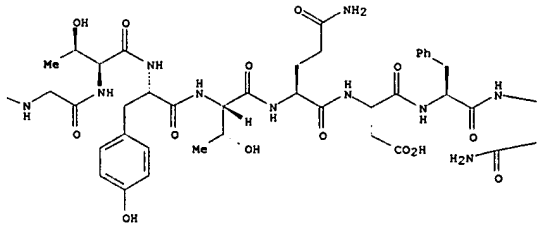
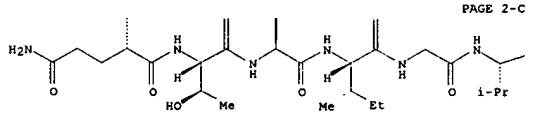


L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-C



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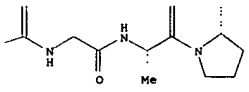

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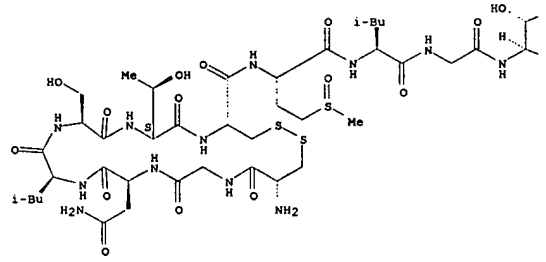
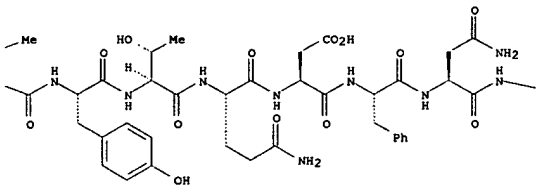
3 STEPS

PAGE 1-A



L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B



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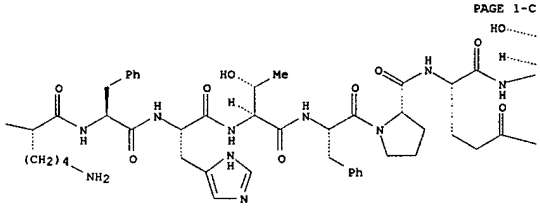

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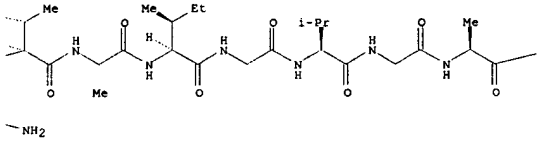
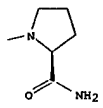


L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-E



AH

RX(1) RCT A 71989-31-6

STAGE(1)
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(2)
RGT U 110-89-4 Piperidine
SOL 68-12-2 DMF

STAGE(3)
RCT B 35661-39-3
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(4)
RCT C 29022-11-5
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(5)
RCT D 68858-20-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(6)
RCT E 71989-23-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(7)
RCT F 73731-37-0
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(8)
RCT G 132327-80-1
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(9)
RGT U 110-89-4 Piperidine

STAGE(10)
RCT H 35661-40-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(11)
RGT U 110-89-4 Piperidine

STAGE(12)
RCT I 109425-51-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(13)
RCT J 105047-45-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(14)
RCT K 132388-59-1
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(15)
RCT L 71989-14-5
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(16)
RCT M 71989-38-3
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(17)
RCT N 35661-60-0
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(18)
RCT O 71989-28-1
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i

L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 68-12-2 DMF

STAGE(19)
RCT P 103213-32-7
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(20)
RCT Q 71989-33-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

PRO R 474527-92-9D
NTE solid-supported reaction, first stage is deprotection of Fmoc-PAL-PEG-PS resin, std. side chains protecting groups (tBu,trityl,Boc) assumed, piperidine used for all subsequent deprotection after coupling

RX(3) RCT R 474527-92-9D, X 474527-93-0D
RGT Z 76-05-1 F3CCO2H, AA 108-95-2 PhOH, AB 100-68-5 PhSMe, AC 540-63-6 HSCH2CH2SH
PRO Y 27686-18-6
SOL 76-05-1 F3CCO2H
NTE solid-supported reaction, other products also detected

RX(2) RCT A 71989-31-6

STAGE(1)
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(2)
RGT U 110-89-4 Piperidine
SOL 68-12-2 DMF

STAGE(3)
RCT B 35661-39-3
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(4)
RCT C 29022-11-5
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(5)
RCT D 68858-20-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(6)
RCT E 71989-23-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,

L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(7)
RCT F 73731-37-0
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(8)
RCT G 132327-80-1
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(9)
RCT H 35661-40-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(10)
RCT I 109425-51-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(11)
RCT J 105047-45-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(12)
RCT K 132388-59-1
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(13)
RCT L 71989-14-5
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(14)
RCT M 71989-38-3
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(15)
RCT N 35661-60-0
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(16)
RCT W 76265-70-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(17)
RCT P 103213-32-7
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(18)
RCT Q 71989-33-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

PRO X 474527-93-0D
NTE solid-supported reaction, first stage is deprotection of Fmoc-PAL-PEG-PS resin, std. side chains protecting groups (tBu,trityl,Boc) assumed, piperidine used for all subsequent deprotection after coupling

RX(2) RCT A 71989-31-6

STAGE(1)
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(2)
RGT U 110-89-4 Piperidine
SOL 68-12-2 DMF

STAGE(3)
RCT B 35661-39-3
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(4)
RCT C 29022-11-5
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(5)
RCT D 68858-20-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

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STAGE(6)
RCT E 71989-23-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(7)
RCT F 73731-37-0
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(8)
RCT G 132327-80-1
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(9)
RCT H 35661-40-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(10)
RCT I 109425-51-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(11)
RCT J 105047-45-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(12)
RCT K 132388-59-1
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(13)
RCT L 71989-14-5
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(14)
RCT M 71989-38-3
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(15)
RCT N 35661-60-0
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(16)
RCT W 76265-70-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(17)
RCT P 103213-32-7
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(18)
RCT Q 71989-33-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

PRO X 474527-93-0D
NTE solid-supported reaction, first stage is deprotection of Fmoc-PAL-PEG-PS resin, std. side chains protecting groups (tBu,trityl,Boc) assumed, piperidine used for all subsequent deprotection after coupling

RX(1) RCT A 71989-31-6

STAGE(1)
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(2)
RGT U 110-89-4 Piperidine
SOL 68-12-2 DMF

STAGE(3)
RCT B 35661-39-3
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(4)
RCT C 29022-11-5
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(5)
RCT D 68858-20-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(6)
RCT E 71989-23-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(7)
RCT F 73731-37-0
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(8)
RCT G 132327-80-1
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(9)
RGT U 110-89-4 Piperidine

STAGE(10)
RCT H 35661-40-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(11)
RGT U 110-89-4 Piperidine

STAGE(12)
RCT I 109425-51-6
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(13)
RCT J 105047-45-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(14)
RCT K 132388-59-1
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(15)
RCT L 71989-14-5
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(16)
RCT M 71989-38-3
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

L62 ANSWER 22 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(17)
RCT N 35661-60-0
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(18)
RCT O 71989-28-1
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(19)
RCT P 103213-32-7
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

STAGE(20)
RCT Q 71989-33-8
RGT S 39968-33-7 3H-1,2,3-Triazolo[4,5-b]pyridine, 3-hydroxy-,
T 693-13-0 i-PrN:C:NPr-i
SOL 68-12-2 DMF

PRO R 474527-92-9D
NTE solid-supported reaction, first stage is deprotection of Fmoc-PAL-PEG-PS resin, std. side chains protecting groups (tBu,trityl,Boc) assumed, piperidine used for all subsequent deprotection after coupling

RX(4) RCT R 474527-92-9D, X 474527-93-0D
RGT Z 76-05-1 F3CCO2H, AB 100-68-5 PhSMe, AC 540-63-6 HSCH2CH2SH, AE
100-66-3 PhOMe
PRO AD 73840-80-9
SOL 76-05-1 F3CCO2H
NTE solid-supported reaction, other products also detected

RX(6) RCT Y 27686-18-6, AD 73840-80-9
RGT AI 12072-77-4 Platinate(2-), dichlorotetrakis(cyano-kC)-, dipotassium, (OC-6-12)-
PRO AH 67881-33-8
NTE buffered soln.

July 8, '02

L62 ANSWER 23 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

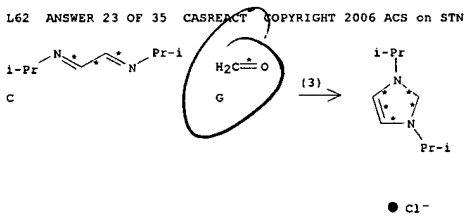
ACCESSION NUMBER: 137:140582 CASREACT
TITLE: Synthesis and Structural Features of Arduengo Carbene Complexes of Group 4 Metallocene Cations
AUTHOR(S): Niehues, Martin; Erker, Gerhard; Kehr, Gerald; Schwab, Pia; Froehlich, Roland; Blacque, Olivier; Berke, Heinz
CORPORATE SOURCE: Organisch-Chemisches Institut, Universitaet Muenster, Muenster, D-48149, Germany
SOURCE: Organometallics (2002), 21(14), 2905-2911
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Treatment of [Cp2TiCH3(THF)+] (5, with [BPh4-] anion) with 1,3-dihydro-1,3-diisopropyl-2H-imidazol-2-ylidene (4; L) at ambient temperature resulted in a rapid displacement of the THF ligand by the stable heterocyclic carbene to yield the Arduengo carbene methyltitanocene cation complex [Cp2TiMeL]BPh4 (6a; >90% isolated). The x-ray crystal structure anal. of 6a showed that the heteroatom-stabilized carbene ligand [d(Ti-C(carbene)) = 2.289(2) Å, d(Ti-CH3) = 2.178(3) Å] was bonded to Ti in an orientation where the imidazol-2-ylidene ring lies in the major σ-ligand plane of the bent metallocene moiety. A DFT calcn. of 6a and related model compds. revealed that the Arduengo carbene serves as a pure σ-donor ligand to the titanocene moiety. The observed favored in-plane orientation of the ligand is steric in origin. Consequently, complex 6a attains an analogous Cs-sym. structure in solution, featuring symmetry-equivalent Cp rings and a pair of diastereotopic iso-Pr substituents as well as chemical differentiated imidazol-2-ylidene C4H:C5H groups. The reaction of the ion pair [(Cp2ZrCH3)+(CH3B(C6F5)3-)] (7) with 4 gave the analogous Arduengo carbene zirconocene cation complex [Cp2ZrMeL]MeB(C6F5)3 (6b; >95% isolated).

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 23 ...C + G ===> H...

L62 ANSWER 23 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



H
YIELD 90%

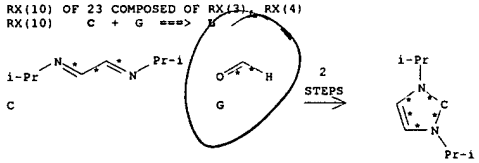
RX(3) RCT C 24764-90-7, G 50-00-0

STAGE(1)
SOL 108-88-3 PhMe

STAGE(2)
RGT I 7647-01-0 HCl
SOL 123-91-1 Dioxane

PRO H 139143-09-2
NTE paraformaldehyde was used

RX(10) OF 23 COMPOSED OF RX(3), RX(4)
RX(10) C + G ===> H



L
YIELD 95%

RX(3) RCT C 24764-90-7, G 50-00-0

STAGE(1)
SOL 108-88-3 PhMe

STAGE(2)
RGT I 7647-01-0 HCl
SOL 123-91-1 Dioxane

PRO H 139143-09-2

L62 ANSWER 23 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
NTE paraformaldehyde was used

RX(4) RCT H 139143-09-2
RGT M 7646-69-7 NaH, N 865-47-4 t-BuOK
PRO L 179863-09-3
SOL 109-99-9 THF

L62 ANSWER 24 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

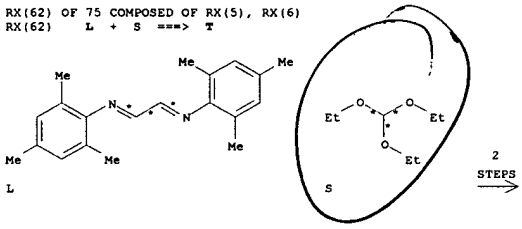
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(5) RCT L 56222-36-7
RGT Q 16940-66-2 NaBH4
PRO P 134030-21-0
SOL 67-56-1 MeOH, 109-99-9 THF

RX(6) RCT P 134030-21-0, S 122-51-0
RGT U 12125-02-9 NH4Cl
PRO T 141556-45-8

L62 ANSWER 24 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 136:69622 CASREACT
TITLE: Amination Reactions of Aryl Halides with Nitrogen-Containing Reagents Mediated by Palladium/Imidazolium Salt Systems
AUTHOR(S): Grasa, Gabriela A.; Viciu, Mihai S.; Huang, Jinkun; Nolan, Steven P.
CORPORATE SOURCE: Department of Chemistry, University of New Orleans, New Orleans, LA, 70148, USA
SOURCE: Journal of Organic Chemistry (2001), 66(23), 7729-7737
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Nucleophilic N-heterocyclic carbenes have been conveniently used as catalyst modifiers in amination reactions involving aryl chlorides, aryl bromides, and aryl iodides with various nitrogen-containing substrates. The scope of a coupling process using a Pd(0) or Pd(II) source and an imidazolium salt in the presence of a base, KOCMe3 or NaOH, was tested using various substrates. The Pd2(dba)3/IPr·HCl [IPr = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene] system presents the highest activity with respect to electron-neutral and electron-rich aryl chlorides. The ligand is also effective for the synthesis of benzophenone imines, which can be easily converted to the corresponding primary amines by acid hydrolysis. Less reactive indoles were converted to N-aryl-substituted indoles using as supporting ligand the more donating SIPr·HCl [SIPr = 1,3-bis(2,6-diisopropylphenyl)-4,5-dihydroimidazol-2-ylidene]. The Pd(OAc)2/SIPr·HCl/NaOH system is efficient for the N-arylation of diverse indoles with aryl bromides. The general protocol developed has been applied successfully to the synthesis of a key intermediate in the synthesis of an important new antibiotic. Mechanistically, palladium-to-ligand ratio studies strongly support an active species bearing one nucleophilic carbene ligand.
REFERENCE COUNT: 114 THERE ARE 114 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

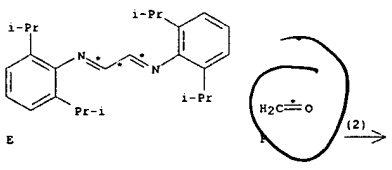
RX(62) OF 75 COMPOSED OF RX(5), RX(6)
RX(62) L + S ===> T



L S

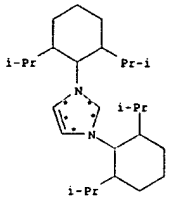
L62 ANSWER 25 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 133:362823 CASREACT
TITLE: A sterically demanding nucleophilic carbene: 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene. Thermochemistry and catalytic application in olefin metathesis
AUTHOR(S): Jafarpour, L.; Stevens, E. D.; Nolan, S. P.
CORPORATE SOURCE: Department of Chemistry, University of New Orleans, New Orleans, LA, 70148, USA
SOURCE: Journal of Organometallic Chemistry (2000), 606(1), 49-54
CODEN: JORCAI; ISSN: 0022-328X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The sterically demanding nucleophilic carbene ligand 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene (IPr, 4) has been synthesized. The reaction of [Cp*RuCl]4 (5; Cp* = η5-C5Me5) with this ligand affords a coordinatively unsatd. Cp*Ru(IPr)Cl (6) complex. Solution calorimetric results in this system provide information concerning the electron donor properties of the carbene ligand. Steric parameters associated with this ligand are determined from the x-ray crystal structure study. The carbene ligand reacts with RuCl2(:C(H)Ph)(PCy3)2 to yield a mixed carbene-phosphine ruthenium complex RuCl2(:C(H)Ph)(IPr)(PCy3) (9). A single-crystal x-ray diffraction study has been performed on 9. The thermal stability of 9 has been studied at 60° and its catalytic activity has been evaluated for the ring closing metathesis of di-Et diallylmalonate.
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 15 ...E + F ===> G...



E F

L62 ANSWER 25 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Cl⁻

G
YIELD 47%

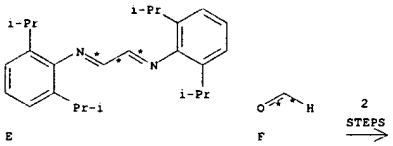
RX(2) RCT E **74663-75-5**, F 50-00-0

STAGE(1)
SOL 108-88-3 PhMe

STAGE(2)
RGT H 7647-01-0 HCl
SOL 123-91-1 Dioxane

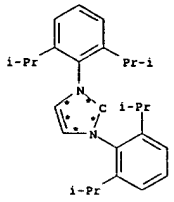
PRO G **250285-32-6**
NTE PARAFORMALDEHYDE USED

RX(7) OF 15 COMPOSED OF RX(2), RX(3)
RX(7) **E + F ===> B**



E F 2 STEPS

L62 ANSWER 25 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



B
YIELD 79%

RX(2) RCT E **74663-75-5**, F 50-00-0

STAGE(1)
SOL 108-88-3 PhMe

STAGE(2)
RGT H 7647-01-0 HCl
SOL 123-91-1 Dioxane

PRO G 250285-32-6
NTE PARAFORMALDEHYDE USED

RX(3) RCT G 250285-32-6
RGT K 865-47-4 t-BuOK
PRO B **244187-81-3**
SOL 109-99-9 THF

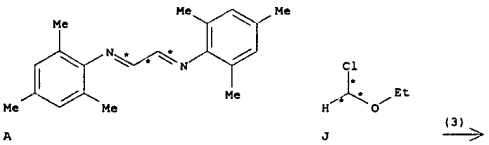
L62 ANSWER 26 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 132:151738 CASREACT
TITLE: Imidazolylidenes, imidazolinylidenes and imidazolidines
AUTHOR(S): Arduengo, Anthony J., III; Krafczyk, Roland; Schmutzler, Reinhard; Craig, Hugh A.; Goerlich, Jens R.; Marshall, William J.; Unverzagt, Markus
CORPORATE SOURCE: Institut fur Anorganische und Analytische Chemie, der Technischen Universitat - Carolo Wilhelmina, Braunschweig, D-38106, Germany
SOURCE: Tetrahedron (1999), 55(51), 14523-14534
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Starting from glyoxal and RNH2 [R = 2,4,6-Me3C6H2, 2,6-(Me2CH)2C6H3], the corresponding 1,3-diarylimidazolinium chlorides were obtained in a 3-step sequence via diimines and ethylenediamine dihydrochlorides. Subsequent reduction with LiAlH4 furnished 1,3-diarylimidazolidines, while their deprotonation with KH in THF gave access to stable carbenes, 1,3-diarylimidazolin-2-ylidenes. Similarly substituted imidazol-2-ylidenes are described for comparison.

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

RX(3) OF 14 **A + J ===> K...**



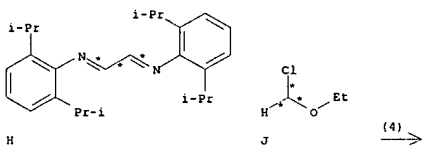
A J (3)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

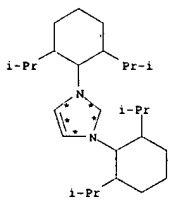
RX(3) RCT A **56222-36-7**, J 3188-13-4
PRO K **141556-45-8**
SOL 109-99-9 THF

RX(4) OF 14 **H + J ===> L...**

L62 ANSWER 26 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



H J (4)

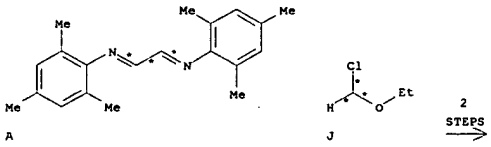


● Cl⁻

L
YIELD 47%

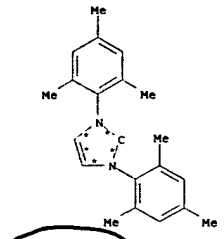
RX(4) RCT H **74663-75-5**, J 3188-13-4
PRO L **250285-32-6**
SOL 109-99-9 THF

RX(9) OF 14 COMPOSED OF RX(3), RX(7)
RX(9) **A + J ===> Q**



A J 2 STEPS

L62 ANSWER 26 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



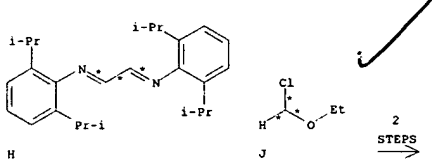
Q
YIELD 96%

yield of deprotonation

RX(3) RCT A **56222-36-7**, J 3188-13-4
PRO K 141556-45-8
SOL 109-99-9 THF

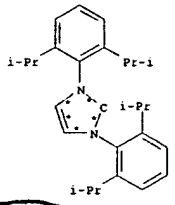
RX(7) RCT K 141556-45-8
RGT N 865-47-4 t-BuOK
PRO Q **141556-42-5**
SOL 109-99-9 THF

RX(10) OF 14 COMPOSED OF RX(4), RX(5)
RX(10) H + J ===> M



H J 2 STEPS

L62 ANSWER 26 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

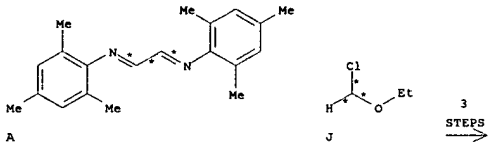


M
YIELD 80%

RX(4) RCT H **74663-75-5**, J 3188-13-4
PRO L 250285-32-6
SOL 109-99-9 THF

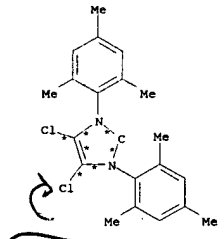
RX(5) RCT L 250285-32-6
RGT N 865-47-4 t-BuOK
PRO M **244187-81-3**
SOL 109-99-9 THF

RX(13) OF 14 COMPOSED OF RX(3), RX(7), RX(8)
RX(13) A + J ===> R



A J 3 STEPS

L62 ANSWER 26 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



R
YIELD 85%

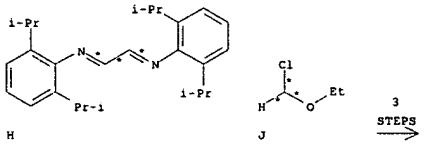
yield of chlorination

RX(3) RCT A **56222-36-7**, J 3188-13-4
PRO K 141556-45-8
SOL 109-99-9 THF

RX(7) RCT K 141556-45-8
RGT N 865-47-4 t-BuOK
PRO Q 141556-42-5
SOL 109-99-9 THF

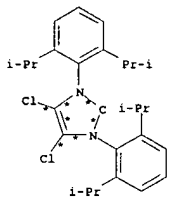
RX(8) RCT Q 141556-42-5
RGT P 56-23-5 CCl4
PRO R **200730-48-9**
SOL 109-99-9 THF

RX(14) OF 14 COMPOSED OF RX(4), RX(5), RX(6)
RX(14) H + J ===> O



H J 3 STEPS

L62 ANSWER 26 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



O
YIELD 77%

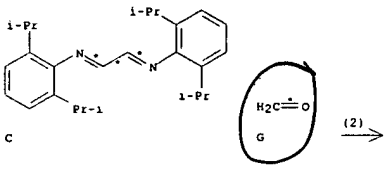
RX(4) RCT H **74663-75-5**, J 3188-13-4
PRO L 250285-32-6
SOL 109-99-9 THF

RX(5) RCT L 250285-32-6
RGT N 865-47-4 t-BuOK
PRO M 244187-81-3
SOL 109-99-9 THF

RX(6) RCT M 244187-81-3
RGT P 56-23-5 CCl4
PRO O **258278-31-8**
SOL 109-99-9 THF

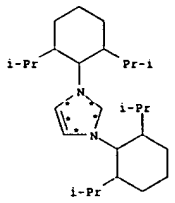
L62 ANSWER 27 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 132:49760 CASREACT
TITLE: Efficient Cross-Coupling of Aryl Chlorides with Aryl Grignard Reagents (Kumada Reaction) Mediated by a Palladium/Imidazolium Chloride System
AUTHOR(S): Huang, Jinkun; Nolan, Steven P.
CORPORATE SOURCE: Department of Chemistry, University of New Orleans, New Orleans, LA, 70148, USA
SOURCE: Journal of the American Chemical Society (1999), 121(42), 9889-9890
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A general methodol. for the Kumada reaction was presented. In the presence of tris[μ-[(1,2-η:4,5-η)-(1E,4E)-1,5-diphenyl-1,4-pentadien-3-one]]dipalladium or palladium diacetate and an imidazolium chloride, aryl chlorides, aryl bromides or aryl iodides underwent a coupling reaction to give biphenyl derivs. Suitable imidazolium compds. were 1,3-bis(2,4,6-trimethylphenyl)-1H-imidazolium chloride and 1,3-bis(2,6-bis(1-methylethyl)phenyl]-1H-imidazolium chloride.
REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 16 ...C + G ===> H



C

L62 ANSWER 27 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

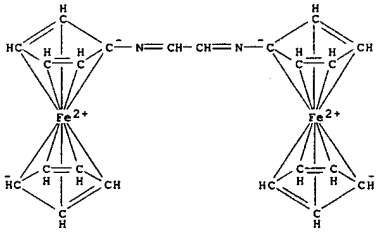


RX(2) RCT C 74663-75-5, G 50-00-0
STAGE(1)
SOL 108-88-3 PhMe
STAGE(2)
RGT I 7647-01-0 HCl
SOL 123-91-1 Dioxane
PRO H 250285-32-6
NTE paraformaldehyde used, prior prepns. were one-pot

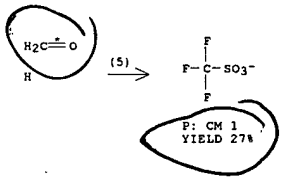
L62 ANSWER 28 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 131:337140 CASREACT
TITLE: N,N'-Diferrocenyl-N-heterocyclic Carbenes and Their Derivatives
AUTHOR(S): Bildstein, Benno; Malaun, Michael; Kopacka, Holger; Wurst, Klaus; Mitterboeck, Martin; Ongania, Karl-Hans; Opromolla, Giuliana; Zanello, Piero
CORPORATE SOURCE: Institut fuer Allgemeine Anorganische und Theoretische Chemie, Universitaet Innsbruck, Innsbruck, A-6020, Austria
SOURCE: Organometallics (1999), 18(21), 4325-4336
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In continuation of the authors' work on Wanzlick/Arduengo carbenes containing redox-active ferrocenyl substituents the synthesis of N,N'-diferrocenyl imidazol(in)ium salts as precursors of imidazol(in)-2-ylidenes is reported. The necessary starting material for this chemical is aminoferrocene, which was prepared by an improved and large-scale synthesis by the sequence solid lithioferrocene, iodoferrocene, N-ferrocenylphthalimide, aminoferrocene. The preparation of N,N'-diferrocenyl heterocycles involves condensation of aminoferrocene with glyoxal to afford N,N'-diferrocenyldiazabutadiene [Fc-DAB], reduction, condensation with formaldehyde, and oxidation with trityl salts to yield N,N'-diferrocenylimidazol(in)ium salts. In situ deprotonation and trapping with electrophiles yielded the expected metal complexes and derivs. in some cases [Ag+ or S8], but attempted reaction with other transition metals [e.g., Pd(II)] failed to give the corresponding complexes, due to (i) steric hindrance by the two N-ferrocenyl substituents, (ii) reduced acidity of the imidazol(in)ium precursors, and (iii) inaccessibility of the free carbenes. Spectroscopic [IR, Raman, UV-visible, MS, NMR (1H, 13C, 109Ag)], structural [x-ray], and electrochem. [CV] properties are reported and compared to those of other N-heterocyclic carbene derivs.
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 66 ...C + O + H ===> P...

L62 ANSWER 28 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

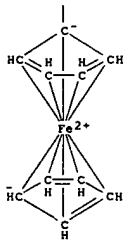


C O



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



P: CM 2
YIELD 27%

L62 ANSWER 28 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

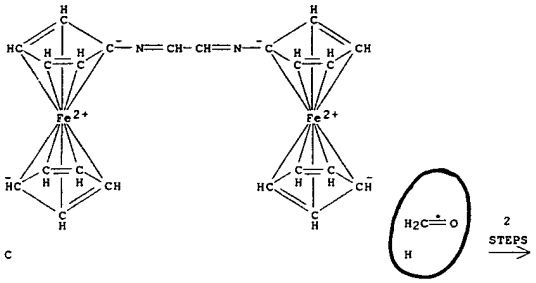
RX(5) RCT C **249644-26-6**, O 1493-13-6

STAGE(1)
RGT Q 557-20-0 Et2Zn
SOL 75-05-8 MeCN, 110-54-3 Hexane

STAGE(2)
RCT H 50-00-0

PRO P **249644-41-5**
NTE PARAFORMALDEHYDE USED

RX(16) OF 66 COMPOSED OF RX(2), RX(3)
RX(16) C + H ===> I



C

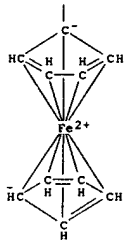
H

2 STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L62 ANSWER 28 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A



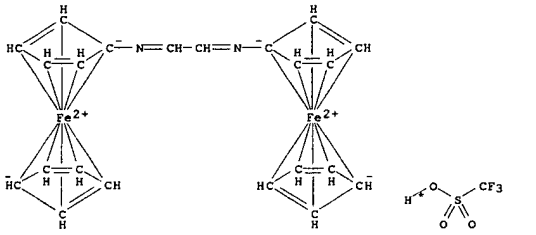
I
YIELD 66%

RX(2) RCT C **249644-26-6**
RGT G 16853-85-3 LiAlH4
PRO F 249644-28-8

RX(3) RCT F 249644-28-8, H 50-00-0
PRO I **249644-30-2**
SOL 67-64-1 Me2CO, 7732-18-5 Water

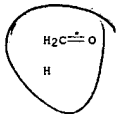
RX(18) OF 66 COMPOSED OF RX(5), RX(6)
RX(18) C + O + H + T ===> U

L62 ANSWER 28 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

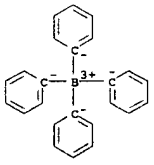


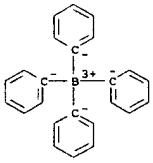
C

O



H





● Na+

T

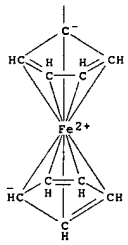
2 STEPS

U: CM 1
YIELD 52%

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L62 ANSWER 28 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A



U: CM 2
YIELD 52%

RX(5) RCT C **249644-26-6**, O 1493-13-6

STAGE(1)
RGT Q 557-20-0 Et2Zn
SOL 75-05-8 MeCN, 110-54-3 Hexane

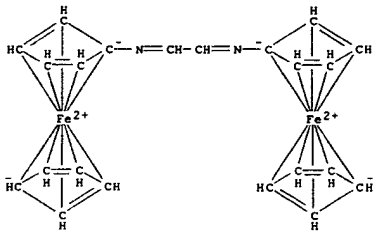
STAGE(2)
RCT H 50-00-0

PRO P 249644-41-5
NTE PARAFORMALDEHYDE USED

RX(6) RCT P 249644-41-5, T 143-66-8
PRO U **249644-43-7**
SOL 67-56-1 MeOH

RX(29) OF 66 COMPOSED OF RX(2), RX(3), RX(13)
RX(29) C + H ===> AO

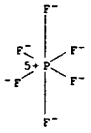
L62 ANSWER 28 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



C

H

3 STEPS

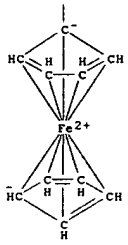


AO: CM 1
YIELD 78%

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L62 ANSWER 28 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A



AO: CM 2
YIELD 78%

RX(2) RCT C **249644-26-6**
RGT G 16853-85-3 LiAlH4
PRO F 249644-28-8

RX(3) RCT F 249644-28-8, H 50-00-0
PRO I 249644-30-2
SOL 67-64-1 Me2CO, 7732-18-5 Water

RX(13) RCT I 249644-30-2
RGT AP 341-02-6 Ph3C.BF4
PRO AO **249644-60-8**
SOL 75-09-2 CH2Cl2

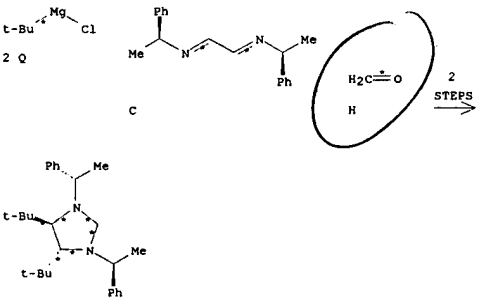
L62 ANSWER 29 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 130:252064 CASREACT
TITLE: A practical and efficient synthesis of enantiomerically pure di-tert-butylethanediamine
AUTHOR(S): Roland, Sylvain; Mangeney, Pierre; Alexakis, Alex
CORPORATE SOURCE: Lab. Chimie Organo-Elements, Univ. Pierre Marie Curie, Paris, F-75252, Fr.
SOURCE: Synthesis (1999), (2), 228-230
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A diastereoselective synthesis of 1,2-di-tert-butylethylenediamine was developed by addition of Me3CMgCl to a chiral bis-imine derived from glyoxal and (S)-α-methylbenzylamine. Addition of the bis-imine to the Grignard reagent in hexane at 50° gave only one diastereomer detectable by 1H and 13C NMR. Hydrogenolysis of the phenylethyl groups led to the expected free (R,R) diamine in good yields.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(7) OF 10 COMPOSED OF RX(4), RX(2)
RX(7) 2 Q + C + H ===> I



I
YIELD 77%

RX(4) RCT Q 677-22-5

STAGE(1)
SOL 60-29-7 Et2O, 110-54-3 Hexane

L62 ANSWER 29 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(2)
RCT C **138812-17-6**
SOL 110-54-3 Hexane

STAGE(3)
RGT R 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO G 221638-36-4
NTE stereoselective

RX(2) RCT G 221638-36-4, H 50-00-0

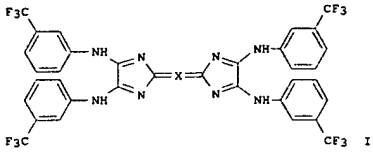
STAGE(1)
RGT E 64-18-6 HCO2H
SOL 7732-18-5 Water

STAGE(2)
RGT J 7732-18-5 Water
SOL 60-29-7 Et2O

STAGE(3)
RGT K 584-08-7 K2CO3

PRO I **221638-37-5**
NTE stereoselective

L62 ANSWER 30 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 129:109035 CASREACT
TITLE: Stable tetraazafulvalenes. Synthesis and chemistry
AUTHOR(S): Kaepplinger, Christian; Beckert, Rainer; Imhof, Wolfgang
CORPORATE SOURCE: Institut Organische Makromolekulare Chemie, Friedrich-Schiller-Universitaet, Jena, D-07743, Germany
SOURCE: Journal fuer Praktische Chemie/Chemiker-Zeitung (1998), 340(4), 323-333
CODEN: JPCCEM; ISSN: 0941-1216
PUBLISHER: Johann Ambrosius Barth
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

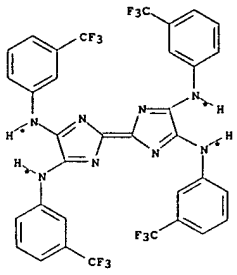


I

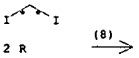
AB The syntheses, properties and reactions of 1,3,6,7-tetrakis(arylamino)-1,4,5,8-tetraazafulvalenes and their vinylogous derivs. are described. The acylation of form- as well as acetamidine with bis-imidoyl chlorides derived from oxalic acid formed reactive cyclic intermediates which dimerized to tetraazafulvalenes I (X = double bond) or bisvinylogous tetraazafulvalenes I [X = (CH)2]. A further synthesis was found using a cycloacylation reaction of amidines with imidoyl chlorides followed by prototropic migration of α-H. Thus, the vinylogous compound I [X = (CH)4] and the phenylogous derivs. I (X = CHC6H4-2-CH, CHC6H4-4-CH) were isolated in moderate to good yields. Besides amidines, other carboxylic acid derivs. such as amides or thioamides were transformed into corresponding tetraazafulvalenes. Due to the vicinal amino groups, alkylation and acylation reactions were studied. For example, the reaction with orthoformates yielded ring-fused products which may be starting material for carbenes just as the cyclization product with SCCl2.
Treatment of tetraazafulvalenes with anhydrous Fe(II) salts or Mo(CO)6 yielded deeply colored metal diazadiene complexes. Finally, reduction using
metallic Li and subsequent alkylation constitutes a convenient synthetic entry to heterocyclic analogs of stilbene.

RX(8) OF 21 Q + 2 R ===> S

L62 ANSWER 30 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

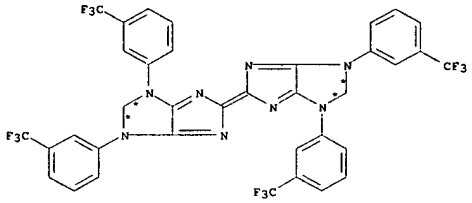


Q



2 R

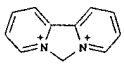
(8)



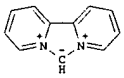
S
YIELD 45%

RX(8) RCT Q 189115-08-0, R 75-11-6
RGT D 121-44-8 Et3N
PRO S 210051-67-5
SOL 1330-20-7 Xylene

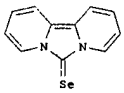
L62 ANSWER 31 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 128:270277 CASREACT
TITLE: Generation and trapping reactions of a formal 1:1 complex between singlet carbon and 2,2'-bipyridine
AUTHOR(S): Weiss, Robert; Reichel, Silvia; Handke, Matthias; Hampel, Frank
CORPORATE SOURCE: Institut fur Organische CHemie, Universitat Erlangen-Nurnberg, Erlangen, D-91054, Germany
SOURCE: Angewandte Chemie, International Edition (1998), 37(3), 344-347
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



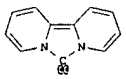
2 OTf⁻ II



X⁻ III



Se IV



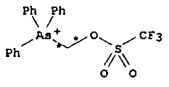
V

AB Treatment of Ph3As+C(=N2)CO2CMe3 with CF3SO3H gave Ph3As+CH2OTf which with
2,2'-bipyridine (I) gave the diquat II which was in equilibrium with its conjugate base III (X- = OTf-); with excess I, II was converted to III (X-
= OTf-). Ion exchange gave 75% III.H2O (X- = Br-) whose crystal structure
was determined III (X- = Br-) in THF containing KOCMe3 and Se gave 100% IV via the
deprotonated singlet C compound V. The crystallog. extensive delocalization
in IV, MO calcns. of III (X- = Br-) and V, isodesmic reactions and reactivity of V, and 13C and 1H NMR of these compds. are discussed.
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

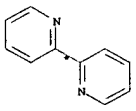
RX(1) OF 5 A + B ===> C...

L62 ANSWER 31 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

A: CM 1

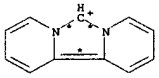


A: CM 2



B

(1)



● Br⁻

C
YIELD 75%

RX(1) RCT A 205182-22-5, B 366-18-7

STAGE(1)
SOL 75-05-8 MeCN

STAGE(2)
SOL 60-29-7 Et2O

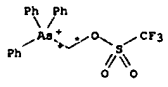
STAGE(3)
RGT D 1643-19-2 Bu4N.Br
SOL 75-09-2 CH2Cl2

PRO C 205182-29-2

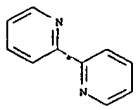
RX(4) OF 5 COMPOSED OF RX(1), RX(2)
RX(4) A + B + H ===> I

L62 ANSWER 31 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

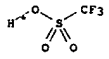
A: CM 1



A: CM 2

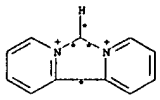


B



H

2 STEPS



I: CM 1
YIELD 90%

I: CM 2
YIELD 90%

RX(1) RCT A 205182-22-5, B 366-18-7

STAGE(1)
SOL 75-05-8 MeCN

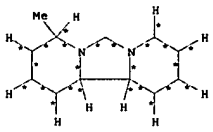
STAGE(2)
SOL 60-29-7 Et2O

STAGE(3)
RGT D 1643-19-2 Bu4N.Br
SOL 75-09-2 CH2Cl2

PRO C 205182-29-2

RX(2) RCT C 205182-29-2, H 1493-13-6
PRO I 205182-23-6
SOL 109-99-9 THF

L62 ANSWER 32 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

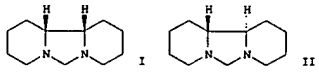


G
YIELD 90%(50)

RX(1) RCT A 56100-22-2
RGT C 1333-74-0 H2
PRO B 23549-50-0
SOL 64-19-7 AcOH

RX(2) RCT E 50-00-0, B 23549-50-0
PRO F 22210-62-4, G 22210-68-0
SOL 7732-18-5 Water

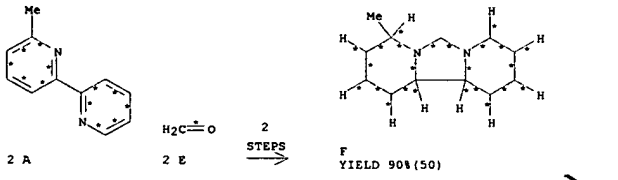
L62 ANSWER 32 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 113:59021 CASREACT
TITLE: Compounds with bridgehead nitrogen. Part 61. Conformational equilibria in the perhydrodipyrido[1,2-c:2',1'-e]imidazoles
AUTHOR(S): Banting, Lee; Crabb, Trevor A.; Fallah, Asadollah; Williams, Roger O.
CORPORATE SOURCE: Dep. Chem., Portsmouth Polytech., Portsmouth/Hampshire, PO1 2DT, UK
SOURCE: Journal of Chemical Research, Synopses (1990), (1), 20
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II

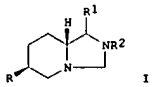
AB syn-Perhydrodipyrido[1,2-c:2',1'-e]imidazole (I) has been shown to adopt an equilibrium in CDCl3 solution at 25 °C between the enantiomeric N-outside-cis-syn-trans-conformers contrary to an earlier report (P. J., Chivers, et al., 1968) assigning a predominance of the trans-syn-trans-conformer. anti-Perhydrodipyrido[1,2-c:2',1'-e]imidazole (II) shows the expected preference for the trans-anti-trans-conformation.

RX(3) OF 3 COMPOSED OF RX(1), RX(2)
RX(3) 2 A + 2 E ===> F + G



2 A 2 E 2 STEPS F
YIELD 90%(50)

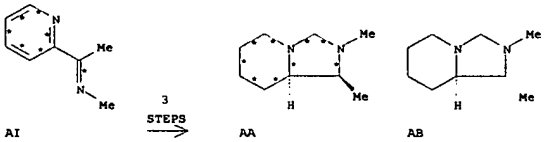
L62 ANSWER 33 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 108:204028 CASREACT
TITLE: Compounds with bridgehead nitrogen. 52. NMR spectra and stereochemistry of the 2-alkylperhydroimidazolo[3,4-a]pyridines
AUTHOR(S): Banting, Lee; Crabb, Trevor A.
CORPORATE SOURCE: Dep. Chem., Portsmouth Polytech., Portsmouth/Hampshire, PO1 2DT, UK
SOURCE: Magnetic Resonance in Chemistry (1987), 25(8), 696-706
CODEN: MRCHEG; ISSN: 0749-1581
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB In contrast to perhydrooxazolo[3,4-a]pyridine and perhydrothiazolo[3,4-a]pyridine, which adopt equilibrium in CDCl3 solution at room temperature containing ca 70% trans fused conformers in equilibrium with O- or S-inside cis fused conformers, 2-alkylperhydroimidazolo[3,4-a]pyridines I [R = R1 = H, R2 = Me, Pr, (CH2)5Me, (CH2)2CHMe(CH2)3CHMe2, CHMe2, cyclohexyl, CMe3; R = Et, R1 = H, R2 = Me, cyclohexyl, CMe3; R = H, R1 = Me, R2 = Me (CH2)5Me, cyclohexyl] are found to adopt equilibrium containing >98% trans fused conformers. Comparison of NMR parameters of I (R = R1 = H, R2 = Me) with those of the 2 isomers of I (R = H, R1 = R2 = Me) indicates an equilibrium for the former compound between the two trans fused conformers, with ca 83% of that conformation containing a trans arrangement of nitrogen lone pairs. These observations are explained in terms of the generalized anomeric effect.

RX(54) OF 62 COMPOSED OF RX(14), RX(28), RX(11)
RX(54) AI ===> AA + AB



AI 3 STEPS AA AB

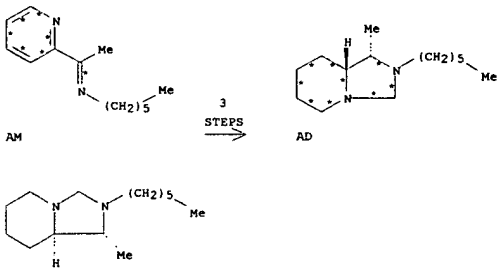
L62 ANSWER 33 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(14) RCT AI **16273-56-6**
RGT AK 16940-66-2 NaBH4
PRO AJ 114366-07-3
SOL 67-56-1 MeOH

RX(28) RCT AJ 114366-07-3
RGT AR 1333-74-0 H2
PRO Z 114366-21-1
CAT 1314-15-4 PtO2
SOL 64-19-7 AcOH

RX(11) RCT Z 114366-21-1
RGT C 50-00-0 HCHO
PRO AA **114365-95-6**, AB 114365-98-9
SOL 7732-18-5 Water

RX(56) OF 62 COMPOSED OF RX(15), RX(29), RX(12)
RX(56) **AM** ===> **AD** + **AE**



AM AD AE

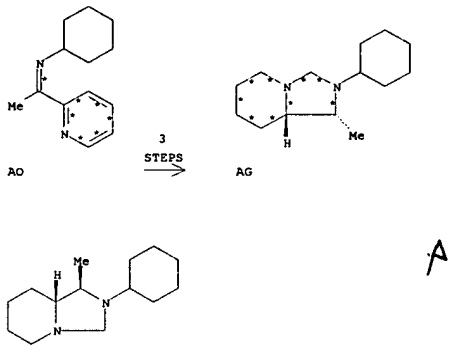
RX(15) RCT AM **114366-24-4**
RGT AK 16940-66-2 NaBH4
PRO AN 114366-08-4
SOL 67-56-1 MeOH

RX(29) RCT AN 114366-08-4
RGT AR 1333-74-0 H2
PRO AC 114366-22-2
CAT 1314-15-4 PtO2
SOL 64-19-7 AcOH

L62 ANSWER 33 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(12) RCT AC 114366-22-2
RGT C 50-00-0 HCHO
PRO AD **114365-96-7**, AE 114365-99-0
SOL 7732-18-5 Water

RX(58) OF 62 COMPOSED OF RX(16), RX(30), RX(13)
RX(58) **AO** ===> **AG** + **AH**



AO AG AH

RX(16) RCT AO **107954-71-2**
RGT AK 16940-66-2 NaBH4
PRO AP 114366-09-5
SOL 67-56-1 MeOH

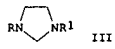
RX(30) RCT AP 114366-09-5
RGT AR 1333-74-0 H2
PRO AF 114366-23-3
CAT 1314-15-4 PtO2
SOL 64-19-7 AcOH

RX(13) RCT AF 114366-23-3
RGT C 50-00-0 HCHO
PRO AG **114365-97-8**, AH 114366-00-6
SOL 7732-18-5 Water

L62 ANSWER 33 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

L62 ANSWER 34 OF 35 CASREACT COPYRIGHT 2006 ACS on STN

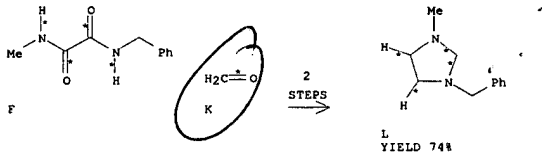
ACCESSION NUMBER: 106:119774 CASREACT
TITLE: Synthesis of 1,3-disubstituted diazolidines
AUTHOR(S): Lambert, Joseph B.; Huseland, Dave E.; Wang, Gen Tai
CORPORATE SOURCE: Dep. Chem., Northwestern Univ., Evanston, IL, 60201, USA
SOURCE: Synthesis (1986), (8), 657-8
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



III

AB Sym. and unsym. RNHCH2CH2NHR1 (I; R = PhCH2, Et, Ph; R1 = Me, Ph, CH2Ph) were obtained by the reduction of RNHCOCONHR1 (II) with LiAlH4. II were readily produced by treatment of di-Et oxalate with primary amines. I gave imidazolidines III on treatment with CH2O.

RX(11) OF 14 COMPOSED OF RX(3), RX(4)
RX(11) **F** + K ===> **L**



F K L
YIELD 74%

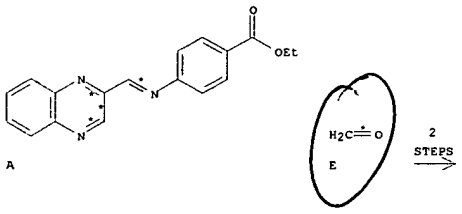
RX(3) RCT F **7666-51-5**
RGT I 16853-85-3 LiAlH4
PRO H 56904-09-7
SOL 109-99-9 THF

RX(4) RCT K 50-00-0, H 56904-09-7
PRO L **105900-08-1**
SOL 64-17-5 EtOH, 7732-18-5 Water

L62 ANSWER 35 OF 35 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 71:101002 CASREACT
TITLE: Models for tetrahydrofolic acid. I. Condensation of formaldehyde with tetrahydroquinoxaline analogs
AUTHOR(S): Benkovic, Stephen J.; Benkovic, Patricia A.; Comfort, David R.
CORPORATE SOURCE: Pennsylvania State Univ., University Park, PA, USA
SOURCE: Journal of the American Chemical Society (1969), 91(19), 5270-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

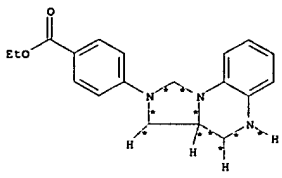
AB To investigate the mechanisms of tetrahydrofolic acid catalyzed one carbon unit transfers, we have synthesized several tetrahydroquinoxaline analogs.
A kinetic investigation of the condensation with CH2O of one of these models reveals the intermediacy of the iminium cation as a steady-state species and the importance of general catalysis in formation of the imidazolidine ring, the latter a model for 5,10-methylene tetrahydrofolic acid. The relevance of these results to the mechanism of one carbon unit transfers and the importance of certain structural and electronic features in the actual cofactor is discussed.

RX(4) OF 4 COMPOSED OF RX(1), RX(3)
RX(4) A + E ===> F



A E

L62 ANSWER 35 OF 35 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



F
YIELD 70%

RX(1) RCT A 62294-77-3
RGT C 16940-66-2 NaBH4
PRO B 23792-11-2
SOL 111-96-6 (MeOCH2CH2)2O
NTE Classification: Chemoselective; Dearomatisation; Reduction; # Conditions: NaBH4; diglyme 1h; 20 deg

RX(3) RCT B 23792-11-2, E 50-00-0
PRO F 25107-69-3
SOL 123-91-1 Dioxane, 7732-18-5 Water
NTE Classification: Heterocycle formation; Condensation; N-Alkylation; # Conditions: 1,4-dioxan H2O; heat water bath